UNIVERSITÀ DI PISA

Appunti di lezione per il corso di
Termofluidodinamica ed Elementi di CFD

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Part II – Elements of Numerical Methods and CFD

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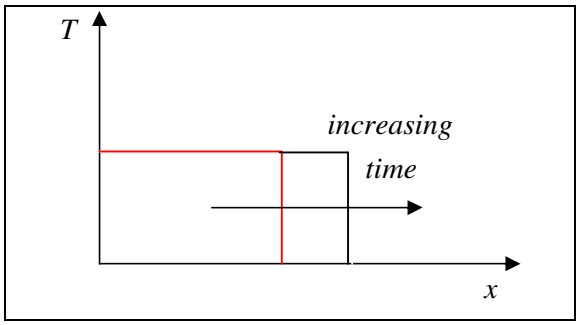
GENERAL CONSIDERATIONS ON NUMERICAL DISCRETIZATION SCHEMES

Mathematical Character of Balance Equations for Fluid Flow

- **The mathematical character of Partial Differential Equations (PDEs) is relevant for their numerical discretization**
  - **the numerical scheme should reflect, though approximately, *the way in which relevant information is propagated throughout the computational domain***
  - ***boundary and initial conditions must be imposed in the numerical method in agreement with the way information is propagated***
- **The classification of PDEs envisages three different characters addressing different phenomena; grossly speaking:**
  - ***hyperbolic*: phenomena involving the propagation of wave fronts progressing along specific space-time paths with finite speed**
  - ***parabolic*: phenomena involving infinite speed of propagation in space and progressing in time**
  - ***elliptic*: steady-state distribution of scalars in space**
- **Examples of *hyperbolic equations***
  - **the advection of a scalar**

$$\frac{\partial T}{\partial t} + w\frac{\partial T}{\partial x} = 0$$



  - **the "vibrating string"**

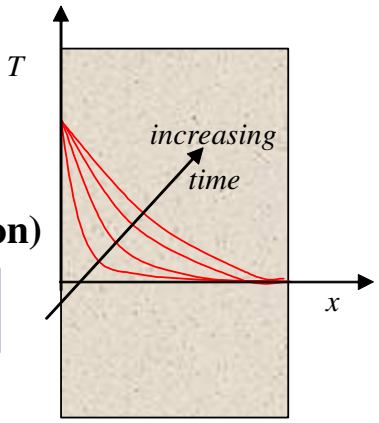
$$\frac{1}{c^2}\frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial x^2} \Rightarrow \qquad T(x,t) = f(x-ct) + g(x+ct)$$

  - **the telegraph equation**

$$\tau\frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2}$$

  - **the compressible Euler equations**

$$\rho\frac{D\vec{w}}{Dt} = -\nabla p + \rho\vec{g}$$

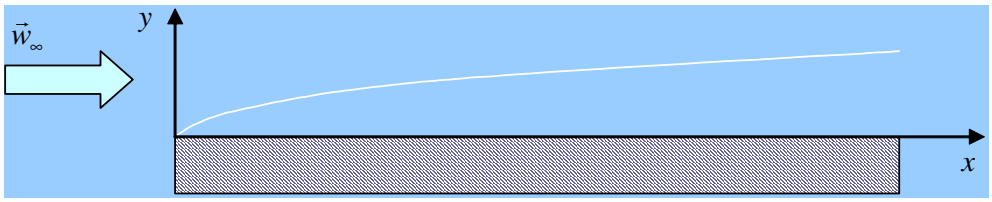


- **Examples of *parabolic equations***
  - **the diffusion of a scalar (heat, concentration)**

$$\frac{\partial T}{\partial t}=\alpha\frac{\partial^2 T}{\partial x^2} \qquad \frac{\partial c}{\partial t}=\mathrm{D}\frac{\partial^2 c}{\partial x^2}$$

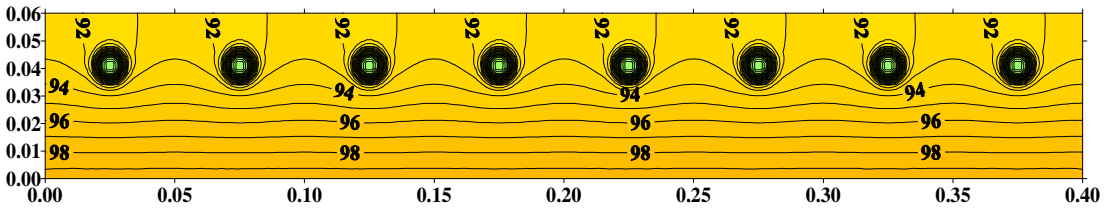
  - **the laminar boundary layer**

$$w_x\frac{\partial w_x}{\partial x}+w_y\frac{\partial w_x}{\partial y}=\nu\frac{\partial^2 w_x}{\partial y^2} \qquad w_x\frac{\partial T}{\partial x}+w_y\frac{\partial T}{\partial y}=\alpha\frac{\partial^2 T}{\partial y^2} \qquad w_x\frac{\partial \omega}{\partial x}+w_y\frac{\partial \omega}{\partial y}=\mathrm{D}\frac{\partial^2 \omega}{\partial y^2}$$



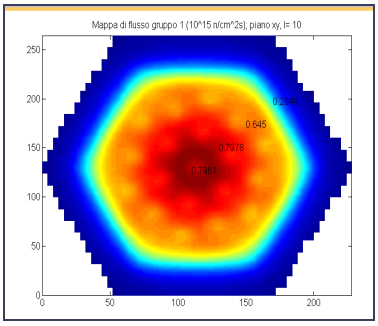
- **Examples of *elliptic equations***
  - **the steady temperature distribution in a solid or the electric potential in a domain**

$$\nabla^2 T=0 \qquad \nabla^2 V=0$$



  - **the steady neutron flux distribution in a reactor core**

$$div\,D_g(\vec{r})\,grad_{\vec{r}}\,\phi_g(\vec{r})-\Sigma_{r,g}(\vec{r})\phi_g(\vec{r})+\sum_{g'<g}\Sigma_{s,g'\to g}(\vec{r})\phi_{g'}(\vec{r})$$
$$+\frac{\chi_g}{k}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(\vec{r})\phi_{g'}(\vec{r})=0 \qquad (\vec{r}\in V,\ g=1,\ldots,G)$$



$$\phi_g(\vec{r})+d_g\frac{d\phi_g(\vec{r})}{dn}=0 \qquad (\vec{r}\in\partial V,\ g=1,\ldots,G)$$

- **Navier-Stokes equations** $\rho\frac{D\vec{w}}{Dt}=\mu\nabla^2\vec{w}-\nabla p+\rho\vec{g}$ **are also elliptic in nature when steady and may be parabolic in transient form**

- **The sets of partial differential equations as the ones describing fluid-dynamics can be classed into hyperbolic, parabolic or elliptic by evaluating their "characteristic roots"**

➢ **the system must be written in the form**

$$\boxed{\mathbf{A}(x,t,\boldsymbol{\varphi})\frac{\partial \boldsymbol{\varphi}}{\partial t}+\mathbf{B}(x,t,\boldsymbol{\varphi})\frac{\partial \boldsymbol{\varphi}}{\partial x}=\mathbf{c}(x,t,\boldsymbol{\varphi})}$$

where $\boldsymbol{\varphi}$ is the vector of unknowns, e.g. $\boldsymbol{\varphi}=\{p,u,w\}$ for single-phase flow and $\boldsymbol{\varphi}=\{p,u_l,u_v,\alpha_v,w_l,w_v\}$ for two-phase flow

➢ **then, the "characteristic equation" is solved**

$$\boxed{\det(\mathbf{B}-\lambda\mathbf{A})=0}$$

- **For the scalar advection equation, $\frac{\partial T}{\partial t}+w\frac{\partial T}{\partial x}=0$, the matrices A and B degenerate into 1 and *w*, giving the characteristic root $\lambda=w$, showing the hyperbolic character of advection.**
- **Generally speaking,**
  - **when the roots of this equation (*characteristic roots)* are real, the system is said *hyperbolic* and the characteristic roots represent the slope of the *characteristic lines* in the *x-t* plane, to be interpreted as the lines along which the relevant information is transported; it is:**

$$\lambda_i=\frac{dx_i}{dt}$$

  - **when all the characteristic roots are complex, the system is said *elliptic*;**
  - **in all the other cases, the system is said *parabolic*.**
- **To better understand the situation, it is worth considering another classification, that can be shown to be equivalent to the above one and applies to second order partial differential equations**

$$a(x,t)\frac{\partial^2\varphi}{\partial t^2}+b(x,t)\frac{\partial^2\varphi}{\partial t\partial x}+c(x,t)\frac{\partial^2\varphi}{\partial x^2}+d(x,t)\frac{\partial\varphi}{\partial t}+e(x,t)\frac{\partial\varphi}{\partial x}+f(x,t)\varphi=g(x,t)$$

The classification is based on the value of $\Delta(x,t)=b^2-4ac$; for $\Delta(x,t)>0$ the equation is *hyperbolic*, for $\Delta(x,t)=b^2-4ac=0$ the equation is *parabolic* and for $\Delta(x,t)=b^2-4ac<0$ the equation is *elliptic*.

- **The relation between the two classifications can be understood considering that the above second order equation can be converted to a system of first order partial differential equations. In fact, by putting**

$$\varphi_1 = \frac{\partial \varphi}{\partial t} \qquad \varphi_2 = \frac{\partial \varphi}{\partial x} \qquad \varphi_3 = \varphi$$

the second order equation can be rewritten as the system of equations

$$\begin{cases} a(x,t)\dfrac{\partial \varphi_1}{\partial t} + b(x,t)\dfrac{\partial \varphi_1}{\partial x} + c(x,t)\dfrac{\partial \varphi_2}{\partial x} + d(x,t)\varphi_1 + e(x,t)\varphi_2 + f(x,t)\varphi = g(x,t) \\ \dfrac{\partial \varphi_2}{\partial t} - \dfrac{\partial \varphi_1}{\partial x} = 0 \\ \dfrac{\partial \varphi_3}{\partial x} - \varphi_2 = 0 \end{cases}$$

- **We have therefore:**

$$\mathbf{A} = \begin{bmatrix} a(x,t) & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} b(x,t) & c(x,t) & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \boldsymbol{\varphi} = \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{bmatrix}$$

and the characteristic equation becomes

$$\det(\mathbf{B} - \lambda \mathbf{A}) = \begin{vmatrix} b(x,t) - \lambda a(x,t) & c(x,t) & 0 \\ -1 & -\lambda & 0 \\ 0 & 0 & 1 \end{vmatrix} = a(x,t)\lambda^2 - b(x,t)\lambda + c(x,t) = 0$$

- **For the vibrating string equation it is**

$$\frac{1}{c^2}\frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial x^2}$$

$$\frac{1}{c^2}\lambda^2 - 1 = 0 \quad \Rightarrow \qquad \lambda_{1,2} = \pm c$$

The equation is therefore hyperbolic and the two characteristic roots represent the speed of propagation of perturbation (waves) along the x axis in the forward and in the backward directions

- **For the telegraph equation, it is**

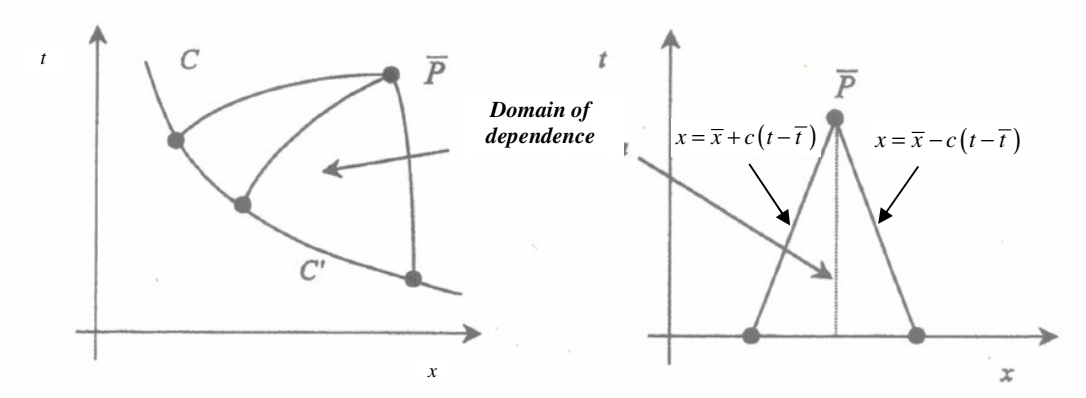
$$\tau\frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2}$$

$$\tau\lambda^2 - \alpha = 0 \quad \Rightarrow \qquad \lambda_{1,2} = \pm\sqrt{\alpha/\tau}$$

So, also this equation is hyperbolic and the two characteristic roots depend on the ratio of the two appearing constants. In both cases, the *real characteristic roots*, represent the speed at which information is

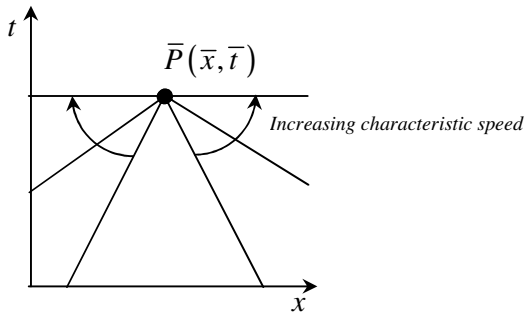
propagated in space during time for hyperbolic phenomena; the *characteristic lines* represent the paths in the space-time plane along which information is propagated: their local slope is given by the characteristic roots

In the figure below, it is clarified that the *"domain of dependence"*, enclosed by the characteristic lines (they may be two and straight, as in the right figure, or more than two and even curved if the characteristic roots are not constant, as in the left one), represents the region from which the state in any given point $\overline{P}$ depends: the relevant information affecting it cannot come from outside the region.



- **The telegraph equation helps in understanding that the speed of propagation of information in the heat equation becomes infinite. In fact, for vanishing τ it is**

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad \underset{\tau \to 0}{\rightarrow} \quad \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$



and the two characteristic roots $\lambda_{1,2} = \pm\sqrt{\alpha/\tau}$ become infinite. This means that any perturbation travels with infinite speed forth and back along the *x* axis, and the domain of dependence is all the region below a certain time $\overline{t}$.

- **For the 2D Laplace equation, it is:**

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \qquad \lambda^2 + 1 = 0$$

and the roots are found to be complex conjugated, showing the elliptic character of the equation.

A RELEVANT EXAMPLE for 1D FLOW ANALYSES

The One-Dimensional Equations for a Compressible Single and Two-Phase Flow

In this approach the single or two-phase fluid is anyway considered as a mixture having cross section averaged properties.

Temperature and velocity are uniquely defined for both phases and the single couple of thermodynamic variables p and u defines the properties of the fluid.

In the case of Two-Phase Flow the model is said HEM (Homogeneous Equilibrium Model) or Equal Velocity Equal Temperature (EVET).

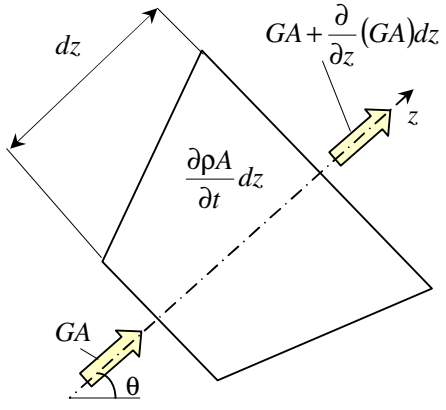
In this respect, the equations to be derived hereafter hold for two-phase mixtures and for single phase fluids as well.

The following equations are written in terms of cross section averaged variables, neglecting the difference between the average of products and the product of averages: this is a simplification often introduced that must anyway be carefully considered in its implications.

- **Mass Balance**

  We consider an elementary duct slice having length equal to dz with cross section area that, in general, can be variable along z

  The mass balance in terms of variables averaged over the cross section can be written as



$$\underbrace{\frac{\partial}{\partial t}(\rho A)\,dz}_{\substack{\text{rate of change}\\ \text{of mass in the volume}}} = \underbrace{GA}_{\substack{\text{inlet mass}\\ \text{flow rate}}} - \underbrace{\left[GA+\frac{\partial}{\partial z}(GA)\,dz\right]}_{\text{outlet mass flow rate}}$$

where $G = W/A = \rho Q/A = \rho w = \left[kg/\left(m^2 s\right)\right]$ ***, is the*** **mass velocity** ***assuming*** w ***as the cross section averaged value of velocity:*** $w = \overline{w}$ **.**

In the case of two-phase flow the **volumetric flux,** j ***, defined as***

$$j = \frac{Q}{A} = \left[\frac{m}{s}\right]$$

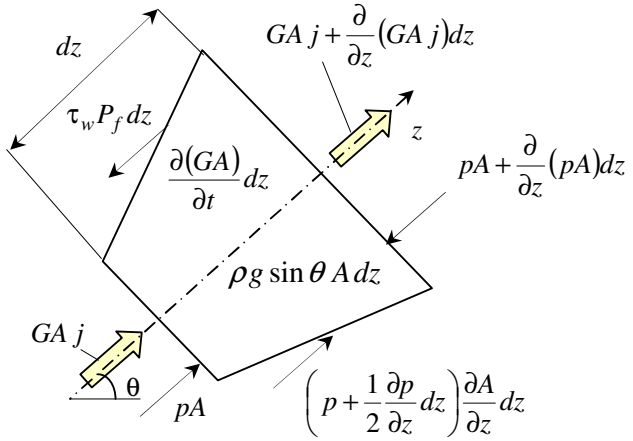
represents a more meaningful definition than $w = \overline{w}$ ***, as it is the speed of the geometrical centre of the mixture.***

By simplifying the differential terms and considering that area is constant in time, it is

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{1}{A}\frac{\partial}{\partial z}(GA) = 0} \qquad \textit{(mass balance)}$$

- **<u>Momentum Balance along the channel axis</u>**

Considering the same elementary volume, **writing again the momentum equation in terms of cross section averaged values** ***it is:***



(P_f ***is the wetted perimeter)***

$$\underbrace{\frac{\partial}{\partial t}(GA)\,dz}_{\substack{\text{rate of change of momentum}\\ \text{in the volume}}} = \underbrace{GA\,j}_{\substack{\text{inlet momentum}\\ \text{flow}}} - \underbrace{\left[GA\,j + \frac{\partial}{\partial z}(GA\,j)\,dz\right]}_{\text{outlet momentum flow}}$$

$$+ \underbrace{pA}_{\substack{\text{pressure force}\\ \text{over the inlet section}}} - \underbrace{\left[pA + \frac{\partial}{\partial z}(pA)\,dz\right]}_{\substack{\text{pressure force}\\ \text{over the outlet section}}}$$

$$+ \underbrace{\left(p + \frac{1}{2}\frac{\partial p}{\partial z}dz\right)}_{\substack{\text{average pressure}\\ \text{at the wall}}} \underbrace{\frac{\partial A}{\partial z}dz}_{\substack{\text{area change}\\ \text{from inlet}\\ \text{to outlet}}} - \underbrace{\tau_w P_f\,dz}_{\substack{\text{friction force}\\ \text{at the wall}}} - \underbrace{\rho g \sin\theta\, A\,dz}_{\text{z component of weight}}$$

Neglecting second order terms and simplifying, it is:

$$\frac{\partial}{\partial t}(GA) = -\frac{\partial}{\partial z}(GA\,j) - \frac{\partial}{\partial z}(pA) + p\frac{\partial A}{\partial z} - \tau_w P_f - \rho g\,sin\,\theta\,A$$

Considering that

$$j = \frac{G}{\rho} \qquad \textbf{and} \qquad \frac{\partial}{\partial z}(pA) = p\frac{\partial A}{\partial z} + A\frac{\partial p}{\partial z}$$

and dividing both sides by the area, it is found

$$\boxed{\frac{\partial G}{\partial t} + \frac{1}{A}\frac{\partial}{\partial z}\left(\frac{G^2 A}{\rho}\right) = -\frac{\partial p}{\partial z} - \rho g\,sin\,\theta - \tau_w\frac{P_f}{A}} \qquad \textbf{(momentum balance)}$$

The previous equation can be also written in the form:

$$\frac{\partial p}{\partial z} = -\underbrace{\frac{\partial G}{\partial t}}_{\substack{temporal\\ acceleration}} \underbrace{-\frac{1}{A}\frac{\partial}{\partial z}\left(\frac{G^2 A}{\rho}\right)}_{\substack{space\\ acceleration}} - \underbrace{\rho g \sin\theta}_{\substack{gravitational\\ term}} - \underbrace{\tau_w\frac{P_f}{A}}_{\substack{friction\\ term}}$$

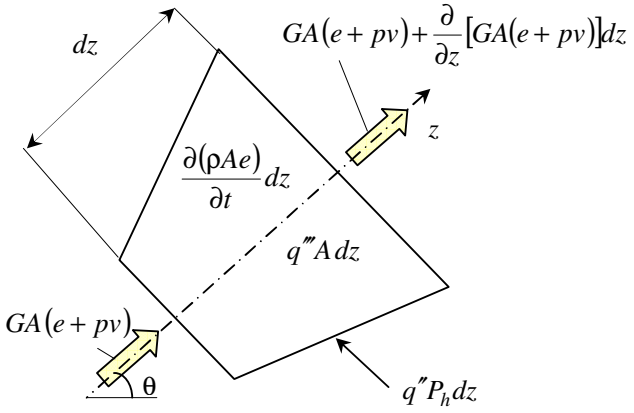
by integrating along a finite length, it is

$$\Delta p = \Delta p_{acc,temp} + \Delta p_{acc,spat} + \Delta p_{grav} + \Delta p_{frict}$$

Obviously, in the case in which singular pressure drops and/or a pump are present, new terms must be introduced, as Δp_{sing} ***e*** Δp_{pump}**.**

- **<u>Energy Balance</u>**

  By taking $e = u + w^2/2 + gz$**, *in terms of variables average over the cress section,* it is:**



$$\underbrace{\frac{\partial}{\partial t}(\rho Ae)\,dz}_{\substack{rate\ of\ change\\ of\ energy\ inside\\ the\ volume}} = \underbrace{GA(e+pv)}_{\substack{thermal\ power\\ +\\ flow\ work\\ at\ the\ inlet}} - \underbrace{\left[GA\,(e+pv) + \frac{\partial}{\partial z}\left[GA\,(e+pv)\right]dz\right]}_{\substack{thermal\ power\\ +\\ flow\ work\\ at\ the\ outlet}} + \underbrace{q''P_h dz}_{\substack{heat\ transfer\\ rate\ at\ the\ wall}} + \underbrace{q'''A dz}_{\substack{power\ generated\\ in\ the\ fluid\ mass}}$$

in which P_h ***is the*** **heated perimeter.** ***It is therefore:***

$$\boxed{\frac{\partial}{\partial t}(\rho e)+\frac{1}{A}\frac{\partial}{\partial z}[GA\,(e+pv)]=q''\frac{P_h}{A}+q'''}$$ ***(energy balance)***

An equivalent form of the equation can be written for single-phase flow making use of the relationship $G=\rho w$ and assuming that the averages of products over the cross sections are equal to the mean of the products (which, as already mentioned, in general is not true):

$$\frac{\partial \rho}{\partial t}+\frac{1}{A}\frac{\partial}{\partial z}(\rho w A)=0$$

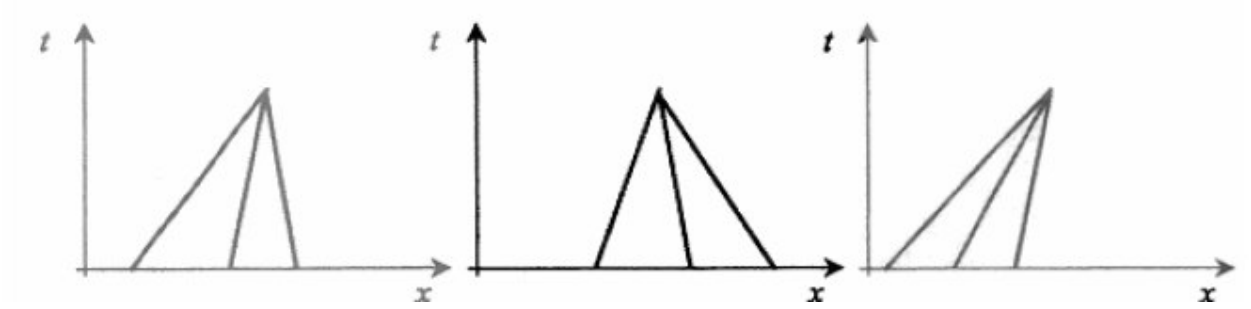
$$\frac{\partial(\rho w)}{\partial t}+\frac{1}{A}\frac{\partial}{\partial z}\left(\rho w^2 A\right)=-\frac{\partial p}{\partial z}-\rho g\,sin\,\theta-\tau_w\frac{P_f}{A}$$

$$\frac{\partial}{\partial t}(\rho e)+\frac{1}{A}\frac{\partial}{\partial z}[\rho w A\,(e+pv)]=q''\frac{P_h}{A}+q'''$$

- **These equations are used also in the case of gas-dynamics along a pipe. A relevant character possessed by these equation is that they are "hyperbolic" having real characteristics (see below)**
- **In the simple Homogeneous Equilibrium Model (HEM), as well as in 1D single-phase compressible flow, the three balance equations lead to three real characteristic roots**

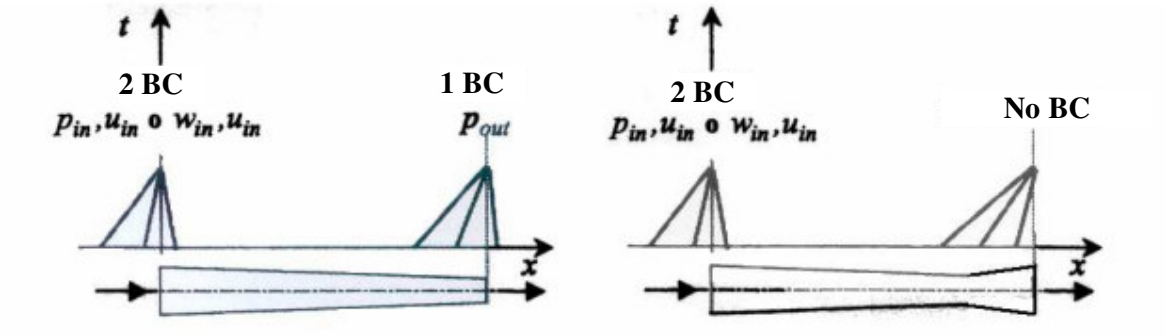
$$\lambda_1 = w + w_{sound} = speed\ of\ \ pressure\ \ perturbations\ in\ the\ \ forward\ direction$$
$$\lambda_2 = w - w_{sound} = speed\ of\ \ pressure\ \ perturbations\ in\ the\ backward\ direction$$
$$\lambda_3 = w = speed\ of\ \ enthalpy\ \ perturbations\ (fluid\ \ velocity)$$

- **The three characteristic lines allow to define the domain of dependence of any point-instant in the space-time plane, highlighting where the needed information on previous time conditions comes from**
- **This is highlighted by the construction of the characteristic line triangles in the following figure**



Subsonic flow towards the right **Subsonic flow towards the left** **Supersonic flow towards the right**

- **Of particular interest is the application of these concepts for determining the type and number of boundary conditions needed at the inlet and at the outlet of a pipe; this is shown in the figure below:**



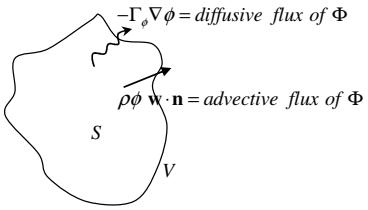
- **On the other hand, for a *six equation two-fluid model*, it is**

$$\lambda_{1,2} = w_f, w_g \qquad \lambda_{3,4} = w_{mixture} \pm w_{void\ \ perturbations} \qquad \lambda_{5,6} = \hat{w}_{mixture} \pm w_{sound}$$

- **Initial value differential problems having an hyperbolic character are "well-posed", because their solution exists and is unique and it changes in a continuous fashion with initial conditions: the latter characteristic is not necessarily possessed by elliptic models**
- **In some cases, *as in the equations adopted by the RELAP5 code, two characteristic roots (the 3rd and 4th in the previous description) generally turn out to be complex giving a partially elliptic character to the equations***
- **The mathematical problem is therefore "ill-posed" and unstable behaviour is possible**
- **In RELAP5, a code used for nuclear reactor application, the problem is anyway *solved at the level of numerical discretization*:**
  - ***by using a numerical scheme introducing enough "numerical diffusion"* as to stabilize the problem**
  - ***by introducing artificial viscosity terms* purposely designed to make sure that a stable solution will be obtained**

The general form of multidimensional balance equations to be solved in fluid dynamics is obtained by conservation principles over arbitrary and finite volumes

$$\underbrace{\frac{d}{dt}\int_V \rho\phi\, dV}_{\substack{\text{Rate of change}\\ \text{of } \Phi \text{ in } V}} = \underbrace{-\int_S \rho\phi\, \mathbf{w}\cdot\mathbf{n}\, dS}_{\substack{\text{Flux of } \Phi \text{ out of } S\\ \text{due to fluid motion}\\ \text{(advection or convection)}}} + \underbrace{\int_S \Gamma_\phi \nabla\phi\cdot\mathbf{n}\, dS}_{\substack{\text{Flux of } \Phi \text{ out of } S\\ \text{due to molecular motion}\\ \text{(diffusion)}}} + \underbrace{\int_V \rho S_\phi\, dV}_{\substack{\text{Volumetric}\\ \text{source of } \Phi}}$$



where ϕ is *the specific value per unit mass of the extensive variable* Φ, being the subject of the balance, and Γ_ϕ and S_ϕ are, respectively, the diffusion coefficient and the source per unit mass

By a conventional passage, the balance equation over the arbitrary volume *V* is firstly transformed by the use of the divergence theorem

$$\underbrace{\int_V \frac{\partial}{\partial t}\rho\phi\, dV}_{\substack{\text{Rate of change}\\ \text{of } \Phi \text{ in } V}} = \underbrace{-\int_V \nabla\cdot(\rho\phi\,\mathbf{w})\, dV}_{\substack{\text{Flux of } \Phi \text{ out of } S\\ \text{due to fluid motion}\\ \text{(advection or convection)}}} + \underbrace{\int_V \nabla\cdot\Gamma_\phi\nabla\phi\ dV}_{\substack{\text{Flux of } \Phi \text{ out of } S\\ \text{due to molecular motion}\\ \text{(diffusion)}}} + \underbrace{\int_V \rho S_\phi\, dV}_{\substack{\text{Volumetric}\\ \text{source of } \Phi}}$$

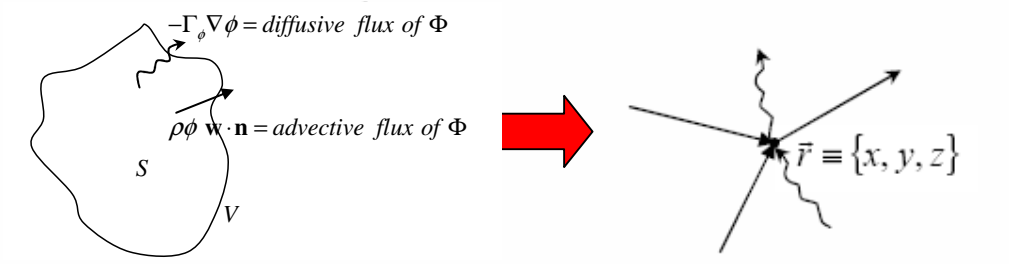
and then the arbitrariness of the selected control volume and the continuity of the functions allows to infer that if

$$\int_V \left[\frac{\partial}{\partial t}(\rho\phi) + \nabla\cdot(\rho\phi\,\mathbf{w}) - \nabla\cdot(\Gamma_\phi\nabla\phi) - \rho S_\phi\right] dV = 0$$

this implies that the integrand function must be zero everywhere:

$$\underbrace{\frac{\partial}{\partial t}(\rho\phi)}_{\text{Transient term}} + \underbrace{\nabla\cdot(\rho\phi\,\mathbf{w})}_{\substack{\text{Advection}\\ \text{(or convection) term}}} = \underbrace{\nabla\cdot(\Gamma_\phi\nabla\phi)}_{\text{Diffusion term}} + \underbrace{\rho S_\phi}_{\text{Source term}}$$

In other words, *the principle of conservation established for a finite volume is translated to the differential (infinitesimal) form*



Since this is the general form of the equations involved in fluid flow, *numerical methods are conceived to deal with the terms appearing in it*.

It will be seen that, making use of the "finite volume" technique of discretization, the red arrow in the previous sketch must be inverted: *from the differential equation we must go back to the finite volume conservation principle.*

BASIC CONCEPTS ABOUT COMPUTATIONAL MODELLING OF TURBULENT FLOWS

LENGTH SCALES IN TURBULENCE

- **In turbulent flow an "energy cascade" occurs representing a transfer of turbulence kinetic energy (per unit mass), identified by *k*, from large to smaller eddies. In particular:**
  - **large eddies receive energy by the average flow field at the macroscopic scales characterising it**
  - **small eddies, on the other hand, are mainly responsible for turbulence kinetic energy dissipation**
  - **it can be reasonably assumed that small eddies are in an equilibrium state in which they receive from large eddies the same rate of energy they dissipate (*universal equilibrium theory* by Kolmogorov, 1941)**
- **Motion at the smaller scales involved in turbulence phenomena is governed by the following variables:**
  - **turbulence kinetic energy dissipation per unit time** $\varepsilon = -dk/dt = \left[m^2/s^3 \right]$
  - **kinematic viscosity** $\nu = \left[m^2/s \right]$
- **By dimensionally combining the above variables, it is possible to determine the *Kolmogorov length, time and velocity scales***

$$\eta \equiv \left(\nu^3/\varepsilon\right)^{1/4} = \left[\left(\frac{m^2}{s} \right)^3 \left(\frac{s^3}{m^2} \right) \right]^{1/4} = \left[m \right]$$

$$\tau \equiv \left(\nu/\varepsilon\right)^{1/2} = \left[\left(\frac{m^2}{s} \right) \left(\frac{s^3}{m^2} \right) \right]^{1/2} = \left[s \right]$$

$$\upsilon \equiv \left(\nu\varepsilon\right)^{1/4} = \left[\left(\frac{m^2}{s} \right) \left(\frac{m^2}{s^3} \right) \right]^{1/4} = \left[\frac{m}{s} \right]$$

- **The length scale η is generally much larger than the mean free paths of molecules; therefore, *turbulent flow is essentially a continuum phenomenon***

- **Nevertheless, *this length scale is many orders of magnitude smaller than that of lager eddies*, whose size is in the order of the length of the bodies which generated them**
- **The length scale characterising large eddies is identified by ℓ and a measure of it is said the *integral turbulence length scale*, representing the distance over which a fluctuating component of velocity keeps "correlated", i.e., such that the mean $\overline{w_i'(\vec{r}_1)\,w_i'(\vec{r}_2)}$ is not negligible for a distance between the two points in the order of ℓ. It is $\ell >> \eta$.**
- **Both on an experimental and on a dimensional basis it was possible to establish the relation between ε, k and ℓ applicable for high Reynolds number turbulence (see later). This relationship has the form**

$$\varepsilon \approx \frac{k^{3/2}}{\ell}$$

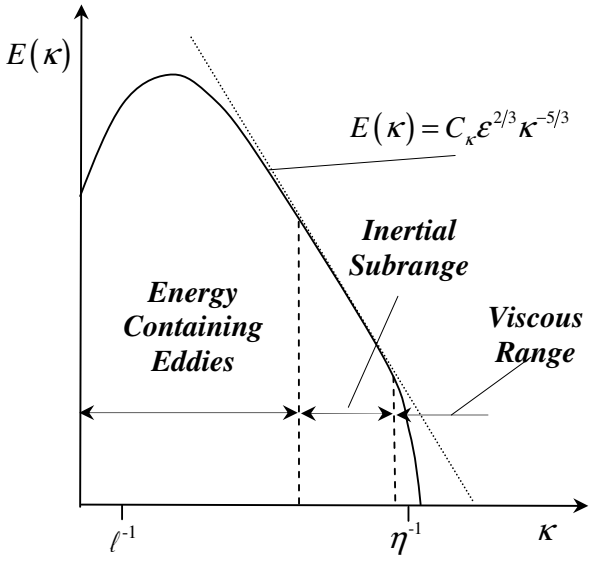
- **Therefore, considering the definition of η it is:**

$$\frac{\ell}{\eta} = \frac{\ell}{\left(\nu^3/\varepsilon\right)^{1/4}} = \frac{\ell\varepsilon^{1/4}}{\nu^{3/4}} \approx \frac{\ell\left(k^{3/2}/\ell\right)^{1/4}}{\nu^{3/4}} = \frac{\ell^{3/4}\left(k^{1/2}\right)^{3/4}}{\nu^{3/4}} = \left[\frac{k^{1/2}\ell}{\nu}\right]^{3/4} = \left(Re_T\right)^{3/4}$$

where $Re_T \equiv \dfrac{k^{1/2}\ell}{\nu}$ is the *turbulence Reynolds number.*

- **Concerning the energy distribution at the different length scales, a spectral distribution originating from a Fourier series decomposition is used**

$$E(\kappa)\,d\kappa = \text{turbulent kinetic energy between } \kappa \text{ and } \kappa + d\kappa$$



with

$k = \frac{1}{2}\left(\overline{w_x'^2} + \overline{w_y'^2} + \overline{w_z'^2}\right) = \int_0^\infty E(\kappa)\,d\kappa$**.**

In this distribution the wave number κ is related to the wavelength, λ, by the relationship $\kappa = 2\pi/\lambda$.

- **The figure shows the qualitative trend of the turbulent energy spectrum <u>in bi-logarithmic scale</u>**

- **Three regions appear:**
  1. **the one of lengths comparable with large eddies, where turbulence takes energy form the mean flow;**
  2. **on the other side, at small values of the wave number, the region of viscous dissipation;**
  3. **the intermediate region, where transfer of energy by inertial mechanisms dominates; in this region, as it has been verified by experiments, the spectrum is proportional to $\varepsilon^{2/3}\kappa^{-5/3}$ (the *Kolmogorov -5/3 law*)**

DIRECT NUMERICAL SIMULATION (DNS)

It is virtually the most accurate method to model turbulent flow. It is based on considering that the Navier-Stokes equations include all the relevant information needed to predict turbulence behaviour

***Direct Numerical Simulation – DNS* does not require special constitutive models for dealing with turbulence; it involves the <u>transient solution</u> of the Navier-Stokes equatons, which model instability phenomena giving rise to eddies; for incompressible flow it is:**

$$\nabla \cdot \vec{w} = 0 \qquad \textit{(continuity equation)}$$

$$\rho \frac{D\vec{w}}{Dt} = \mu \nabla^2 \vec{w} - \nabla p + \rho \vec{g} \qquad \textit{(Navier-Stokes equations)}$$

In this light, *DNS can be thought as a source of data having the same worth of experimental ones*:

- **making use of accurate numerical techniques (for instance, spectral or pseudo-spectral methods), it allows to reproduce with reasonable accuracy phenomena as the onset of turbulence and its characteristics;**
- **it allows to obtain more detailed data than any experiment will ever be able to provide.**

However, beware:

<u>Nothing can really substitute experience!!!</u>

The main problem involved in DNS is that the direct solution of Navier-Stokes equations should be sufficiently accurate over the whole range of involved lengths

This results in a formidable computational problem, since all the involved lengths scales should be adequately resolved (from the

Kolmogorov microscale, η, to the integral length scale, being in the order of the size of the duct or the flow surrounded object):

- **an estimate of the number of equally spaced nodes necessary in this purpose in a duct having an height H is available (Wilcox 1998 book) and is in the order $10^6 \div 10^9$ increasing with $(Re_\tau)^{9/4}$, where $Re_\tau = w_\tau (H/2)/\nu$ and $w_\tau = \sqrt{\tau_w/\rho}$;**
- **similarly, the time step should be in the order of the time scale τ, giving rise to a very large number of time advancements;**

For these reasons, DNS is presently an interesting tool for research, under continuous development, but its applications are limited by the present computer capabilities.

LARGE EDDY SIMULATION (LES)

In the attempt to overcome the problem of resolving the small scales of turbulence, LES methods have been proposed, having the following characteristics:

- **the large turbulence scales are directly solved as in DNS;**
- **the smaller scales are treated with subgrid models (SGS – SubGrid Scale).**

In some relevant cases, the LES technique allowed to obtain results similar to those of DNS with a computational effort in the order of some percentage in terms of required number of nodes and time advancements.

A key point in LES is the choice of a technique to <u>filter</u> the small scales; different options are available:

- ***"volume-average box filter"***

$$\overline{w}_i(\vec{r},t) = \frac{1}{V(\vec{r})} \int_{V(\vec{r})} w_i(\vec{r}',t)\, dV'$$

where it is

$$V(\vec{r}) \equiv \{x - \Delta x/2 \le x' \le x + \Delta x/2,\ y - \Delta y/2 \le y' \le y + \Delta y/2,\ z - \Delta z/2 \le z' \le z + \Delta z/2\}$$

(V is a parallelepiped *"box"*, having sides $\Delta x, \Delta y, \Delta z$ around $\vec{r}$); in this case, $\overline{w}_i$ is the *resolvable-scale filtered velocity*, representing the velocity scale which can be resolved numerically

Obviously, it is:

$$w_i = \overline{w}_i + w_i'$$

formally similar to the relationships applicable in the case of RANS on the basis of time averages that, in this case, is based on the selected spatial averaging process; $\Delta = \sqrt[3]{\Delta x \, \Delta y \, \Delta z}$ **is said the *filter width* and** w_i' **and the *subgrid-scale velocity***

- ***"filter functions"***

  in this case filter functions $G(\vec{r} - \vec{r}', \Delta)$ **are introduced; they give**

$$\overline{w}_i(\vec{r}, t) = \int_{V(\vec{r})} G(\vec{r} - \vec{r}', \Delta) \, w_i(\vec{r}', t) \, dV'$$

  and satisfy the obvious normalization condition:

$$\int_{V(\vec{r})} G(\vec{r} - \vec{r}', \Delta) \, dV' = 1$$

  There are different possible choices:

  - ***"volume-average box filter"***

$$G(\vec{r} - \vec{r}', \Delta) = \begin{cases} 1/V(\vec{r}), & r \in V(\vec{r}) \\ 0, & otherwise \end{cases}$$

  - ***"Gaussian filter"***

$$G(\vec{r} - \vec{r}', \Delta) = \left(\frac{6}{\pi \Delta^2} \right)^{3/2} \exp\left(-6 \frac{|\vec{r} - \vec{r}'|^2}{\Delta^2} \right)$$

  - ***filters based on the Fourier transform (spectral methods)***

    once the velocity field is expressed in terms of wave number κ **(i.e., the reciprocal of a length scale) it is possible to impose that the filter cuts all the components characterised by a wave number greater than a threshold** $\kappa_{\max} = 2\pi/\Delta$ **; an example of such technique is the following *"Fourier cutoff filter"*:**

$$G(\vec{r} - \vec{r}', \Delta) = \frac{1}{V(\vec{r})} \frac{\sin\left[(x - x')/\Delta\right]}{(x - x')/\Delta} \frac{\sin\left[(y - y')/\Delta\right]}{(y - y')/\Delta} \frac{\sin\left[(z - z')/\Delta\right]}{(z - z')/\Delta}$$

Once the *resolvable scales* and the *subgrid scales* have been defined, the Navier-Stokes equations, making use of the Einstein notation (the repeated index in a term implies summation over all the applicable values of such index), can be written in averaged form:

$$\frac{\partial \overline{w}_i}{\partial x_i} = 0 \qquad \textbf{\textit{(continuity)}}$$

$$\frac{\partial \overline{w}_i}{\partial t} + \frac{\partial \overline{w_i w_j}}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{w}_i}{\partial x_k \partial x_k} \qquad \textbf{\textit{(momentum)}}$$

The average appearing as an argument of the derivative in the second term at the LHS can be decomposed as follows:

$$\overline{w_i w_j} = \overline{\left(\overline{w}_i + w_i'\right)\left(\overline{w}_j + w_j'\right)} = \overline{\overline{w}_i \overline{w}_j} + \overline{\overline{w}_i w_j'} + \overline{\overline{w}_j w_i'} + \overline{w_i' w_j'}$$

or (note that in general: $\overline{\overline{w'}} \neq \overline{w'}$)

$$\overline{w_i w_j} = \overline{w}_i \overline{w}_j + \underbrace{\left(\overline{\overline{w}_i \overline{w}_j} - \overline{w}_i \overline{w}_j\right)}_{L_{ij}=Leonard\ stress} + \underbrace{\overline{\overline{w}_i w_j'} + \overline{\overline{w}_j w_i'}}_{C_{ij}=cross-term\ stress} + \underbrace{\overline{w_i' w_j'}}_{R_{ij}=SGS\ Reynolds\ stress}$$

The *Leonard stress* is often implicitly represented by the truncation error of the numerical scheme, if it is a second order one, otherwise it must be directly evaluated. It is also possible to show that

$$L_{ij} \propto \nabla^2\left(\overline{w}_i \overline{w}_j\right)$$

Nevertheless, by adopting the notation:

$$\tau_{ij} = -\left(\overline{w_i w_j} - \overline{w}_i \overline{w}_j\right)$$

or, alternatively, putting

$$\tau_{ij} = -\left(Q_{ij} - \frac{1}{3} Q_{kk} \delta_{ij}\right) \qquad P = \overline{p} + \frac{1}{3}\rho Q_{kk} \delta_{ij} \qquad Q_{ij} = C_{ij} + R_{ij}$$

we have finally an equation having the form:

$$\frac{\partial \overline{w}_i}{\partial t} + \frac{\partial \overline{w}_i \overline{w}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu \frac{\partial \overline{w}_i}{\partial x_j} + \tau_{ij}\right]$$

The above relationship shows that *the fundamental problem in LES is the determination of a model for the <u>subgrid stresses</u>,* τ_{ij} .

Smagorinski in 1963 proposed a relatively successful subgrid model based on the definition of an *eddy viscosity*, ν_T such that

$$\tau_{ij} = 2\nu_T S_{ij}$$

with

$$\nu_T = (C_S \Delta)^2 \sqrt{S_{ij} S_{ij}} \qquad\qquad S_{ij} = \frac{1}{2}\left(\frac{\partial \overline{w}_i}{\partial x_j} + \frac{\partial \overline{w}_j}{\partial x_i} \right)$$

where C_S is the Smagorinski coefficient representing a parameter to be adjusted for the particular problem to be dealt with; values in the range 0.10 to 0.24 have been adopted for typical problems.

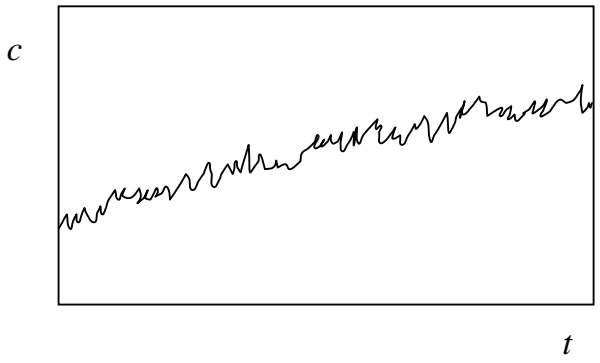
In some more recent *dynamic* subgrid scale models C_S is updated at each advancement.

The LES models require particular care in imposing the boundary conditions, being virtually suitable for the use beyond the viscous boundary layer, at large Reynolds number.

LES models are promising for design applications, though they are still heavy from the computational point of view.

REYNOLDS AVERAGED NAVIER-STOKES EQUATIONS (RANS)

- **Turbulent flow is characterised by the *chaotic* fluctuation of variables (velocity, pressure, temperature, etc.) around mean values that may be also variable (more slowly) in time**



- **A description of the instantaneous behaviour of the fluid is of limited interest for engineering purposes**
- **It is therefore preferable to describe the change in time or space of average values, adopting a statistical treatment for fluctuations**
- **The average value of the intensive variable c is therefore defined by the relationship**

$$\overline{c}(t)=\frac{1}{\Delta t}\int_{t-\Delta t/2}^{t+\Delta t/2} c(\tau)\, d\tau$$

and the instantaneous value of c is decomposed in the summation of the average and the *fluctuating value, having a zero time average*

$$c(t)=\overline{c}(t)+c'(t) \qquad \textbf{and} \qquad \int_{t-\Delta t/2}^{t+\Delta t/2} c'(\tau)\, d\tau = 0$$

- **The time interval adopted in averaging Δt must be chosen long enough to "filter" the turbulent fluctuations, but short enough to avoid jamming the longer term variation of average quantities**
- **The extent of fluctuations can be quantified by their quadratic averages: $\overline{c'^2}$**
- **As a particular case, let us consider the quantities**

$\sqrt{\overline{w_i'^2}}$ ***turbulence intensity for the i-th velocity component***

$\sqrt{\overline{w_x'^2}+\overline{w_y'^2}+\overline{w_z'^2}}$ ***turbulence intensity***

$\overline{w_i' w_j'}$ $(i, j = x, y, z)$ ***double correlation***

- ***Turbulent intensity* is strictly related to the *turbulent kinetic energy***

$$k=\frac{1}{2}\left(\overline{w_x'^2}+\overline{w_y'^2}+\overline{w_z'^2}\right)$$

The time (Reynolds) averaging applied to the Navier-Stokes equations leads to the following expression:

$$\frac{\partial}{\partial t}\left(\rho\,\overline{\vec{w}}\right)+\nabla\cdot\left(\rho\,\overline{\vec{w}}\,\overline{\vec{w}}\right)=\nabla\cdot\left(\overline{\vec{\tau}}-\overline{p}\vec{I}\right)+\rho\vec{g}-\nabla\cdot\left(\rho\,\overline{\vec{w}'\vec{w}'}\right)$$

where

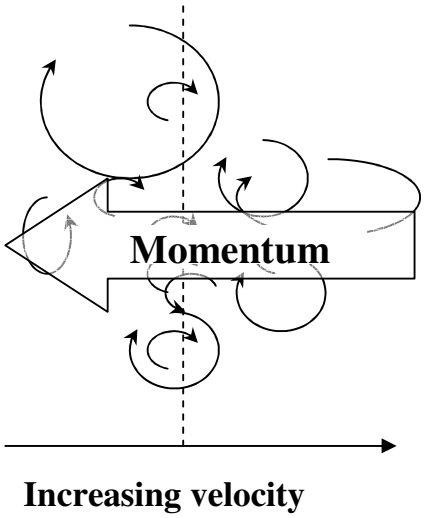
$$\vec{\tau}^{t}=\vec{\tau}_{Re}=-\rho\,\overline{\vec{w}'\vec{w}'}$$

is the *Reynolds stress tensor*.

***This tensor is the main quantity to be simulated in turbulence flows by the RANS approach*, since it represents the additional momentum flux due to turbulence.**

The *Boussinesq approximation* allows making use of the concept of *eddy viscosity*, ν_T, for evaluating this stress in similarity with formulations adopted for laminar flow

$$\tau_{ij} = 2\rho\nu_T S_{ij} = \rho\nu_T \left(\frac{\partial \overline{w}_i}{\partial x_j} + \frac{\partial \overline{w}_j}{\partial x_i} \right)$$



- **Different models have been proposed to calculate this stress. They can be distinguished in the following categories:**
  1. **Algebraic models (or *zero-equation* models)**
  2. **One-equation models**
  3. **Two-equation models**
- **The complexity of these models is greater the larger is the number of "equations" (i.e., *partial differential equations, PDEs*) that must be added to the averaged mass, energy and momentum balance equations (RANS); in particular:**
  - ***no additional PDE is added in algebraic models*;**
  - ***one or two PDEs are added in one-equation and two-equation models*.**
- **"Stress transport models", on the other hand, do not make use of the Boussinesq approximation, defining transport equations for each of the six independent components of the turbulent stress tensor**
- **With respect to algebraic models, the *models with one or more equations allow specify the transport of kinetic energy*, so that the *previous and upstream history* of the flow is accounted for in addition to local conditions**

- **An important distinction between turbulence models is anyway the one between *complete and incomplete models*:**
  - **completeness of the model is related to *its capability to automatically define a characteristic length of turbulence***
  - ***in a complete model, therefore, only the initial and boundary conditions are specified, with no need to define case by case parameters depending on the particular considered flow***

Algebraic Models

Prandtl mixing length theory (1925)

As we already saw, Prandtl assumed that the turbulent stress tensor could be defined by

$$\tau_{yx}^{t} = \rho\, l_{mix}^{2} \left|\frac{\partial \overline{w}_x}{\partial y}\right| \frac{\partial \overline{w}_x}{\partial y}$$

where l_{mix} is the mixing length; the model is similar to the one for molecular viscosity in which kinematic viscosity is a interpreted as the product of a mean molecular velocity by a length (the mean free path).

It is an incomplete model, since the mixing length is different according to the particular flow (boundary layers, jets, wakes, …).

In the case of a wall, Prandtl assumed l_{mix} to be linearly dependent on the distance from the wall, by a law having the form $l_{mix} = Cy$, with C and empirical constant. In the case of a jet or of the mixing between two streams at different velocity ("mixing layer") l_{mix} is proportional to the width of the jet or of the mixing layer, i.e., to the width of the zone in which velocity is sufficiently different from the one of the free unperturbed stream.

Notwithstanding its simplicity, the mixing length model provides reasonable results in a reasonable number of conditions, after being reasonably tuned for the particular flow.

Some of the variants to the model have been:

- **the introduction by Van Driest (1956) of a damping function**

$$l_{mix} = \kappa y\left[1 - e^{-y^{+}/A_0^{+}}\right] \qquad A_0^{+} = 26$$

$\kappa = 0.41$ *von Karman constant* **improving the behaviour of the Reynolds stress at $y^{+} \to 0$, in agreement with theoretical predictions ($\tau_{yx} \sim y^{4}$);**

- **a modification introduced by Clauser (1956) in order to improve the representation of turbulent viscosity in the defect layer;**
- **the introduction of two different formulations for turbulent viscosity in the "inner layer" and the "outer layer" (*two-layer models* by Cebeci-Smith, 1967, and Baldwin-Lomax, 1978);**
- **the introduction of an ordinary differential equation to define turbulent viscosity in the outer layer in two-layer models (*1/2 equation models* by Johnson and King, 1985, and Johnson and Coakley, 1990)**

Algebraic models, anyway, though they have some attractiveness for their simplicity, require being "tuned" to the particular flow to be predicted.

In this light, they must be considered incomplete, in the above specified meaning of this word.

Partial Differential Equation Models

A look to the stress transport equations

Though the stress transport models do not fall in the considered category (they are actually *beyond the Boussinesq approximation*), they are the starting point to understand the derivation of the turbulence kinetic energy equation

Following the treatment for an incompressible fluid (v. Wilcox, 1998), it is:

- **the general component of the Navier-Stokes equation can be written as**

$$N\left(w_i\right) = \rho\frac{\partial w_i}{\partial t} + \rho w_k\frac{\partial w_i}{\partial x_k} + \frac{\partial p}{\partial x_i} - \mu\frac{\partial^2 w_i}{\partial x_k \partial x_k} = 0 \qquad (i,k = x,y,z) \quad (^1)$$

- **considering the identity**

$$N\left(w_i\right)w_j' + N\left(w_j\right)w_i' = 0 \qquad \left(i,j = x,y,z\right)$$

and applying to it the time-averaging operator, it is:

$$\overline{N\left(w_i\right)w_j' + N\left(w_j\right)w_i'} = 0 \qquad \left(i,j = x,y,z\right) \qquad (°)$$

- **the same techniques and assumptions adopted in deriving the RANS equations lead now to equations for each stress tensor component; for instance, consider the transient term in the Navier-Stokes equations:**

(1) **The Einstein's notation is again adopted.**

$$\rho\left[\overline{w_j'\frac{\partial\left(\overline{w}_i+w_i'\right)}{\partial t}+w_i'\frac{\partial\left(\overline{w}_j+w_j'\right)}{\partial t}}\right]=\rho\left[\overline{w_j'\frac{\partial\overline{w}_i}{\partial t}+w_j'\frac{\partial w_i'}{\partial t}+w_i'\frac{\partial\overline{w}_j}{\partial t}+w_i'\frac{\partial w_j'}{\partial t}}\right]$$

$$=\rho\left[\overline{w_j'\frac{\partial\overline{w}_i}{\partial t}}+\overline{w_j'\frac{\partial w_i'}{\partial t}}+\overline{w_i'\frac{\partial\overline{w}_j}{\partial t}}+\overline{w_i'\frac{\partial w_j'}{\partial t}}\right]=\rho\left[\underbrace{\overline{w_j'}}_{=0}\frac{\partial\overline{w}_i}{\partial t}+\overline{w_j'\frac{\partial w_i'}{\partial t}}+\underbrace{\overline{w_i'}}_{=0}\frac{\partial\overline{w}_j}{\partial t}+\overline{w_i'\frac{\partial w_j'}{\partial t}}\right]$$

$$=\rho\left[\overline{w_j'\frac{\partial w_i'}{\partial t}}+\overline{w_i'\frac{\partial w_j'}{\partial t}}\right]=\rho\overline{\frac{\partial\left(w_i'w_j'\right)}{\partial t}}=\rho\frac{\partial\left(\overline{w_i'w_j'}\right)}{\partial t}=-\rho\frac{\partial\tau_{ij}}{\partial t}$$

where, on the contrary of the notation adopted up to now, from here on τ_{ij} identifies the *"specific" Reynolds stress tensor*, defined as

$$\tau_{ij}=-\overline{w_i'w_j'}$$

(differing from the usual notation $\tau_{ij}=-\rho\overline{w_i'w_j'}$).

By proceeding in a similar way, term by term, from (°) it is:

$$\frac{\partial\tau_{ij}}{\partial t}+\overline{w}_k\frac{\partial\tau_{ij}}{\partial x_k}=-\tau_{ik}\frac{\partial\overline{w}_j}{\partial x_k}-\tau_{jk}\frac{\partial\overline{w}_i}{\partial x_k}+2\nu\overline{\frac{\partial w_i'}{\partial x_k}\frac{\partial w_j'}{\partial x_k}}+\overline{\frac{w_i'}{\rho}\frac{\partial p'}{\partial x_j}}+\overline{\frac{w_j'}{\rho}\frac{\partial p'}{\partial x_i}}+\frac{\partial}{\partial x_k}\left[\nu\frac{\partial\tau_{ij}}{\partial x_k}+\overline{w_i'w_j'w_k'}\right]$$

This equation shows the typical difficulties encountered when trying to "close" the turbulence equations. In fact:

- **the application of the time-averaging operator to the Navier-Stokes equations makes the Reynolds stress tensor to appear as a tensor of "correlation" between two fluctuating velocity components ($\overline{w_i'w_j'}$);**
- **the derivation of transport equations for the Reynolds stress tensor makes higher order correlation terms to appear: ($\overline{w_i'w_j'w_k'}$).**

This endless process can be therefore "closed" only including "closure laws" for the unknown terms at some stage. **In the Reynolds stress transport equations the unknown terms became a lot:**

- **10 unknown terms having the form $\overline{w_i'w_j'w_k'}$**
- **6 unknown terms having the form $\overline{\frac{w_i'}{\rho}\frac{\partial p'}{\partial x_j}}+\overline{\frac{w_j'}{\rho}\frac{\partial p'}{\partial x_i}}$**
- **6 unknown terms having the form $2\nu\overline{\frac{\partial w_i'}{\partial x_k}\frac{\partial w_j'}{\partial x_k}}$**

The turbulence kinetic energy equation

The turbulence kinetic energy equation can be now obtained by taking the trace of the equations for the specific transport of Reynolds stress tensor components (i.e., taking the summation of the diagonal terms). In fact:

$$\tau_{ii} = -\overline{w_i' w_i'} = -\left(\overline{w_x'^2} + \overline{w_y'^2} + \overline{w_z'^2}\right) = -2k$$

Its classical form is:

$$\underbrace{\frac{\partial k}{\partial t}}_{\substack{\text{unsteady}\\ \text{term}}} + \underbrace{\overline{w}_j \frac{\partial k}{\partial x_j}}_{\substack{\text{convective}\\ \text{term}}} = \underbrace{\tau_{ij} \frac{\partial \overline{w}_i}{\partial x_j}}_{\text{production}} - \underbrace{\nu \overline{\frac{\partial w_i'}{\partial x_k} \frac{\partial w_i'}{\partial x_k}}}_{\text{dissipation}} + \frac{\partial}{\partial x_j}\left[\underbrace{\nu \frac{\partial k}{\partial x_j}}_{\substack{\text{molecular}\\ \text{diffusion}}} - \underbrace{\frac{1}{2}\overline{w_i' w_i' w_j'}}_{\substack{\text{turbulent}\\ \text{transport}}} - \underbrace{\frac{1}{\rho}\overline{p' w_j'}}_{\substack{\text{pressure}\\ \text{diffusion}}}\right]$$

where the various terms are:

- **<u>unsteady term</u>: as in every balance equation, it represents the local change rate of the quantity to be conserved;**
- **<u>convective (or advective) term</u>: it represents the turbulence kinetic energy transport due to the mean fluid motion;**
- **<u>production term</u>: it represents the transfer of energy from the mean flow per unit time; the Reynolds stress appearing in it is evaluated by:**

$$\boxed{\tau_{ij} = 2\nu_T S_{ij} - \frac{2}{3} k \delta_{ij} = \nu_T \left(\frac{\partial \overline{w}_i}{\partial x_j} + \frac{\partial \overline{w}_j}{\partial x_i}\right) - \frac{2}{3} k \delta_{ij}}$$

  where ν_T is the turbulent diffusivity of momentum (eddy viscosity);

- **<u>dissipation term</u>: it represents the rate at which the turbulence kinetic energy is converted into thermal internal energy; on the basis of dimensional considerations, it is defined as:**

$$\varepsilon = \nu \overline{\frac{\partial w_i'}{\partial x_k} \frac{\partial w_i'}{\partial x_k}}$$

  and is approximated by relationships having the form

$$\varepsilon \sim \frac{k^{3/2}}{\ell}$$

- **<u>molecular diffusion term</u>: it represents the diffusive transport due to processes occurring at a molecular level;**
- **<u>turbulent transport term</u>: it represents the contribution to the kinetic energy transport due to the velocity turbulent fluctuations;**

- **<u>pressure diffusion term</u>: it is the term due to the correlation existing between pressure and velocity fluctuations.**

Turbulent and pressure diffusion transport terms are sometimes grouped together and represented with a single term:

$$\frac{1}{2}\overline{w_i' w_i' w'}_j + \frac{1}{\rho}\overline{p' w_j'} \approx -\frac{\nu_T}{\sigma_k}\frac{\partial k}{\partial x_j}$$

in which σ_k is a parameter correlating turbulent diffusivity of momentum to that of turbulence kinetic energy. It is therefore:

$$\frac{\partial k}{\partial t} + \overline{w}_j \frac{\partial k}{\partial x_j} = \tau_{ij}\frac{\partial \overline{w}_i}{\partial x_j} - \varepsilon + \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]$$

<u>One-Equation Models</u>

Prandtl (1945) proposed to express dissipation rate as

$$\varepsilon = C_D \frac{k^{3/2}}{\ell}$$

However, in this way, the integral turbulence length scale must be defined, for instance, on the basis of approaches similar to those adopted for the mixing length theory.

The one-equation model by Prandtl takes therefore the form

$$\frac{\partial k}{\partial t} + \overline{w}_j \frac{\partial k}{\partial x_j} = \tau_{ij}\frac{\partial \overline{w}_i}{\partial x_j} - C_D \frac{k^{3/2}}{\ell} + \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]$$

A further closure equation is defined for the turbulent viscosity

$$\nu_T = k^{1/2}\ell = C_D \frac{k^2}{\varepsilon}$$

More complex models have been proposed later on, though they refer to similar expressions.

In general, *one-equation models are incomplete*, since the turbulence length scale must be defined on a case by case basis; complete versions are anyway available which specify independently this length (e.g., Baldwin-Barth, 1990).

<u>Two-equation models</u>

As we saw, one-equation models, though they introduce the transport equation for turbulence kinetic energy, are generally incomplete, since they do not define explicitly the turbulence length scale

In order to solve this problem, different two-equation approaches have been proposed:

- **Kolmogorov in 1942 proposed that a new equation for the transport of the *specific dissipation rate,* $\omega = \left[s^{-1} \right]$, dimensionally related to the other quantities by the relationships:**

$$\nu_T \sim k/\omega \qquad \ell \sim k^{1/2}/\omega \qquad \varepsilon \sim \omega k$$

- **Chou in 1945 proposed the introduction of an exact equation for ε, related to the other quantities by**

$$\nu_T \sim k^2/\varepsilon \qquad \ell \sim k^{3/2}/\varepsilon \qquad \omega \sim \varepsilon/k$$

- **Zeierman and Wolfstein in 1986 proposed an equation for the transport of the product of *k* and the turbulence dissipation time, τ, which is essentially the reciprocal of Kolmogorov's ω; it is:**

$$\nu_T \sim k\tau \qquad \ell \sim k^{1/2}\tau \qquad \varepsilon \sim k/\tau$$

From these proposals the so-called $k-\omega$, $k-\varepsilon$ and $k-k\tau$ where obtained. Other proposed models where the $k-k\ell$ (Rotta, 1951).

A short description of the $k-\omega$ and $k-\varepsilon$ models follows, since they were the ones that received the greatest attention up to the present time.

$k-\omega$ *Model*

Kolmogorov defined ω *as "the rate of dissipation of energy per unit volume and unit time".* He underlined its relation with the turbulence length scale, defining ω as a mean frequency given by

$$\omega = c\, k^{1/2}/\ell$$

where *c* is a constant.

Most of considerations by Kolmogorov in relation to ω and its transport equation were based on dimensional reasoning; in his work there is no formal derivation of the equation for ω.

Wilcox (1998) proposed in the following way the possible steps of Kolmogorov's reasoning in identifying ω as a variable whose transport evaluation is needed:

- **also basing on the Boussinesq approximation, it is reasonable to assume that eddy viscosity is proportional to the turbulent kinetic energy: $\nu_T \propto k$;**
- **as $\nu_T = \left[m^2/s \right]$ and $k = \left[m^2/s^2 \right]$, their ratio has the dimension of a time;**
- **similarly, $\varepsilon = \left[m^2/s^3 \right]$ and then $\varepsilon/k = \left[1/s \right]$**

- **we can therefore close from a dimensional point of view the relationships between the different quantities by defining a variable having the dimension of a time or of its reciprocal.**

Then, to define an equation for ω we can assume that the essential terms that it must contain must represent the *time rate of change, convection (advection) diffusion, dissipation, dispersion and production*

The equation, in the form proposed by Kolmogorov, was:

$$\frac{\partial \omega}{\partial t} + \overline{w}_j \frac{\partial \omega}{\partial x_j} = -\beta \omega^2 + \frac{\partial}{\partial x_j}\left[\sigma \nu_T \frac{\partial \omega}{\partial x_j} \right]$$

From the original formulation by Kolmogorov, the $k-\omega$ model was subjected to different developments. The Wilcox (1998) version is the following:

$$\frac{\partial k}{\partial t} + \overline{w}_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial \overline{w}_i}{\partial x_j} - \beta^* k \omega + \frac{\partial}{\partial x_j}\left[\left(\nu + \sigma^* \nu_T \right) \frac{\partial k}{\partial x_j} \right]$$

$$\frac{\partial \omega}{\partial t} + \overline{w}_j \frac{\partial \omega}{\partial x_j} = \alpha \frac{\omega}{k} \tau_{ij} \frac{\partial \overline{w}_i}{\partial x_j} - \beta \omega^2 + \frac{\partial}{\partial x_j}\left[\left(\nu + \sigma \nu_T \right) \frac{\partial \omega}{\partial x_j} \right]$$

with additional formulations for the appearing constants.

For dissipation, turbulent viscosity and the turbulence characteristic length scale in this model it is:

$$\varepsilon = \beta^* k \omega \qquad \nu_T = k/\omega \qquad \ell = k^{1/2}/\omega$$

The coefficients appearing in the above equations are all defined on the basis of laws which do not include any arbitrary assumption of the relevant parameters (v. Wilcox, 1998, Sect. 4.3.1): *the model is therefore complete*.

$k-\varepsilon$ *Model*

It is the most often used turbulence model. The so-called standard $k-\varepsilon$ model was presented in a fundamental paper by Jones and Launder (1972).

Launder and Sharma in 1974 made a retuning of the model, so also their paper is often taken as reference.

Unlike the equation for ω, the transport equation for ε may be obtained by a rigorous process based on the Navier-Stokes equations

$$N(w_i) = \rho \frac{\partial w_i}{\partial t} + \rho w_k \frac{\partial w_i}{\partial x_k} + \frac{\partial p}{\partial x_i} - \mu \frac{\partial^2 w_i}{\partial x_k \partial x_k} = 0 \qquad (i,k = x,y,z)$$

by developing the following identity:

$$2\nu\overline{\frac{\partial w_i'}{\partial x_j}\frac{\partial}{\partial x_j}\left[N\left(w_i\right)\right]}=0$$

The development is relatively complex and leads to an equation including at the RHS the following terms: *production of dissipation, dissipation of dissipation, molecular diffusion of dissipation and turbulent transport of dissipation.*

The equations of the *standard* $k-\varepsilon$ *model* are:

$$\frac{\partial k}{\partial t}+\overline{w}_j\frac{\partial k}{\partial x_j}=\tau_{ij}\frac{\partial \overline{w}_i}{\partial x_j}-\varepsilon+\frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]$$

$$\frac{\partial \varepsilon}{\partial t}+\overline{w}_j\frac{\partial \varepsilon}{\partial x_j}=C_{\varepsilon 1}\frac{\varepsilon}{k}\tau_{ij}\frac{\partial \overline{w}_i}{\partial x_j}-C_{\varepsilon 2}\frac{\varepsilon^2}{k}+\frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]$$

where

$$\nu_T=C_\mu k^2/\varepsilon \qquad \omega=\varepsilon/\left(C_\mu k\right) \qquad \ell=C_\mu k^{3/2}/\varepsilon$$

and the constants are given by:

$$C_{\varepsilon 1}=1.44 \qquad C_{\varepsilon 2}=1.92 \qquad C_\mu=0.09 \qquad \sigma_k=1 \qquad \sigma_\varepsilon=1.3$$

As it is seen, also this model is *complete*.

In summary:

- **by two-equation models, after evaluating the couple $k-\varepsilon$ *or* $k-\omega$, *the eddy viscosity* ν_T *is evaluated*:**

  $$\nu_T=C_\mu k^2/\varepsilon \qquad \textbf{or} \qquad \nu_T=k/\omega$$

  allowing to calculate the Reynolds stress tensor, by the Boussinesq approximation

  $$\tau_{ij}=2\nu_T S_{ij}-\frac{2}{3}k\delta_{ij}=\nu_T\left(\frac{\partial \overline{w}_i}{\partial x_j}+\frac{\partial \overline{w}_j}{\partial x_i}\right)-\frac{2}{3}k\delta_{ij}$$

- **when accepting the Reynolds analogy between heat and momentum transfer, *a prescribed value of the turbulent Prandtl number (often close to unity) allows for the calculation of the thermal eddy diffusivity***

  $$Pr_t=\frac{\nu_T}{\alpha_T}\approx 1$$

  necessary to evaluate the turbulent contribution in energy averaged equations

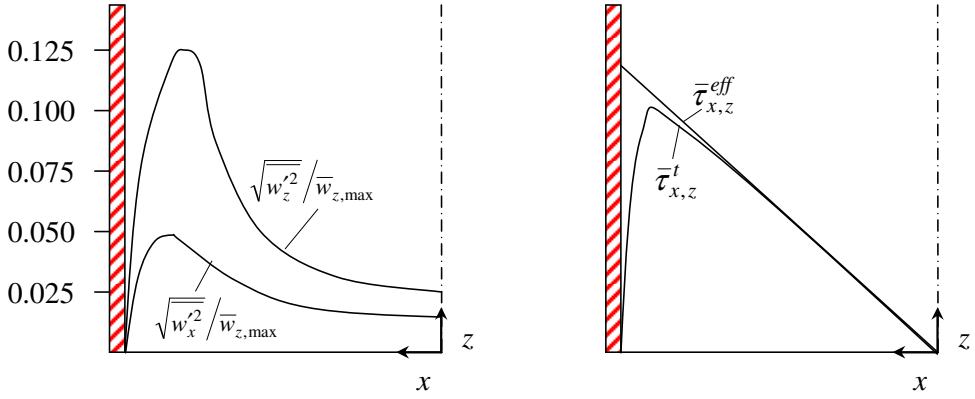
Concluding remarks

- **It can be noted that also the equations of two-equation models can be put in the general conservation form**

$$\frac{\partial}{\partial t}(\rho\phi)+\frac{\partial}{\partial x_j}\left(\rho w_j\phi\right)=\frac{\partial}{\partial x_j}\Gamma_\phi\frac{\partial\phi}{\partial x_j}+S_\phi$$

  to be discretised *with the same numerical techniques adopted for general balance equations* and described in the first part of this lecture

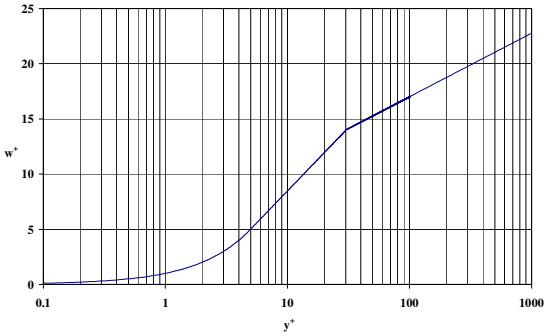
- **It is quite difficult to catch turbulent phenomena close to the wall, *because of the sharp gradients of turbulence intensity*, that are difficult to be described with enough detail**



- **This is the reason why the application of $k-\omega$ and $k-\varepsilon$ turbulence models close to the wall requires attention, because *standard models cannot be integrated up to the wall, where turbulence is damped in the buffer and laminar sublayer regions***

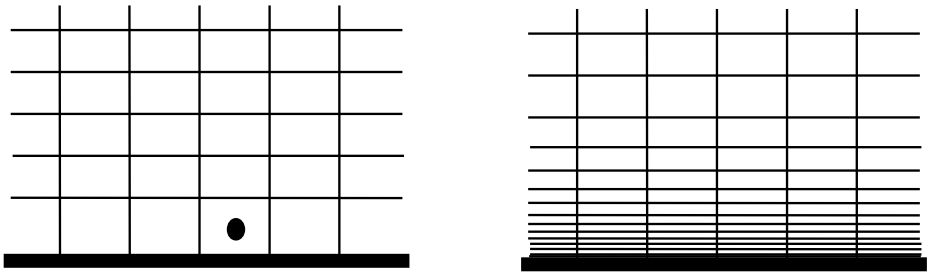
  In this regard, *two possible choices are presently available*:

  - **the use of *"wall functions"*, adopting the well known logarithmic form of the velocity profile to obtain the appropriate boundary conditions to be imposed in the first node close to the wall; in this case, the first node must be put at a large enough value of y^+ (e.g., greater than 30)**



with $w_\tau=\sqrt{\frac{\tau_w}{\rho}}$ $\qquad w_z^+\left(y^+\right)=\frac{w_z(y)}{w_\tau}$ $\qquad y^+=\frac{w_\tau y}{\nu}$

- **as an alternative, *low Reynolds number models* must be used, in which corrections aiming at a better evaluation of the viscous effects close to the wall are introduced (by *"damping functions"*). In this case, the first node close to the wall must be put at $y^+ < 1$, well within the laminar sublayer: *a very refined mesh is necessary at the walls***



(a) Wall functions mesh (b) Low-Reynolds number mesh

- **For a compressible fluid, the averaging process to be adopted is the so-called *Favre averaging*, consisting in averaging the different variables using density as the weight; for instance for velocity it is:**

$$\tilde{w}_i = \frac{1}{\bar{\rho}} \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} \rho w_i \, dt$$

- **On the basis of this definition, it is possible to define the conservation equations averaged according to Favre for mass, energy and momentum as the equations for the Reynolds stress tensor components and of turbulence kinetic energy**
- **The latter is given by:**

$$\frac{\partial}{\partial t}\left(\bar{\rho}k\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{w}_j k\right) = \bar{\rho}\tau_{ij}\frac{\partial \tilde{w}_i}{\partial x_j} - \bar{\rho}\varepsilon + \frac{\partial}{\partial x_j}\left[\overline{t_{ij}u_i''} - \overline{\rho u_j''\frac{1}{2}u_i''u_i''} - \overline{p'u_j''}\right] - \overline{u_i''\frac{\partial P}{\partial x_i}} + \overline{p'\frac{\partial u_i''}{\partial x_i}}$$

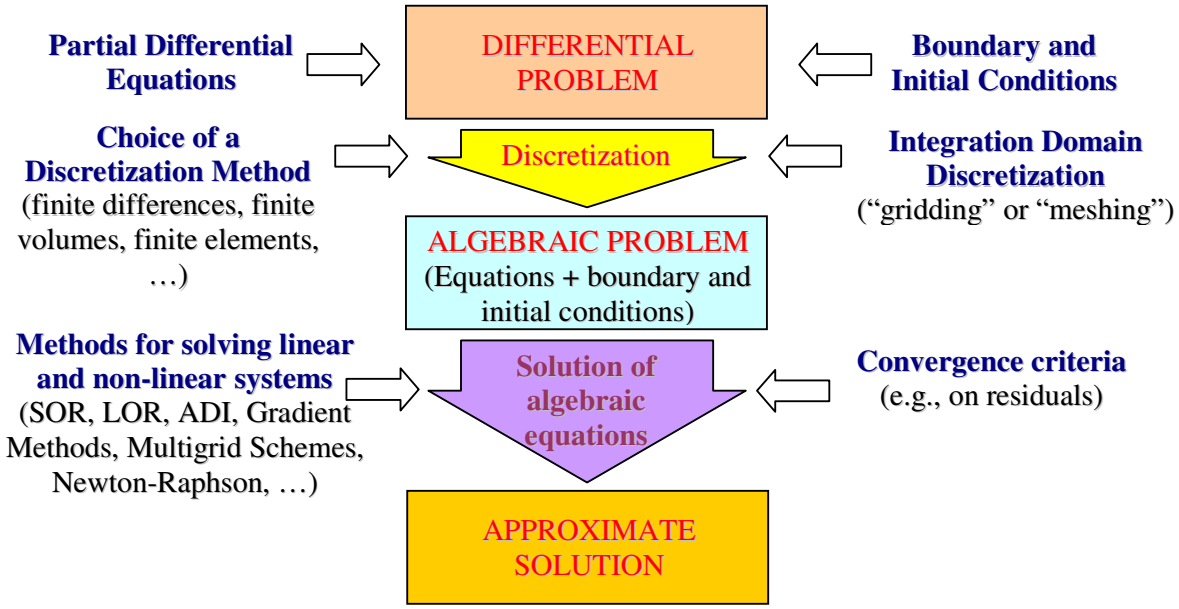
where

$$t_{ij} = 2\mu s_{ij} - \frac{2}{3}\mu\frac{\partial w_k}{\partial x_k}\delta_{ij} \qquad p = P + p' \qquad w_i = \tilde{w}_i + w_i''$$

The last two terms appearing in the *k* equation are *pressure work* and *pressure dilatation.*

NUMERICAL DISCRETIZATION METHODS

- **Partial Differential Equations applicable to engineering problems can be seldom solved in closed form: a phase of *discretization* and *numerical solution* is generally necessary**
- **This *discretization process represents a quite important phase* in partial differential equation system solution. Its major phases can be described as follows:**



Discretizing a partial differential equation problem having engineering interest is therefore *the process of translating the mathematical problem from the continua of space and time to a discrete subset of them, where the solution is evaluated in a point-wise fashion*

The *most common discretization schemes* refer to the following techniques:

- **<u>finite differences</u>: strictly speaking, the partial derivatives in the governing equations are substituted with expressions based on finite differences of the independent variable and of the space and time increments:**

***→ algebraic equations in the nodal values of the unknown variable are obtained*;**

- **<u>finite volumes</u>: the governing equations are integrated over *control volumes* in which the overall domain is subdivided, in order to resume the conservation principle they were derived from; making use of particular definitions of the volume and the surface integrals**

  → *algebraic equations in the nodal values of the unknown variable are obtained*;

- **<u>finite elements:</u> local approximating functions depending on values of the unknown variables in the nodes of the *elements* in which the space is subdivided are optimised by the use of the "method of weighted residuals":**

  → *algebraic equations in the nodal values of the unknown variable are obtained*.

So, *whatever the adopted numerical discretization method, the final problem is to deal with systems of algebraic equations* that must be solved (generally by iterative solution methods)

These algebraic equations must have specific mathematical properties that we have to carefully take into account

We must clarify that even if these properties will be mainly described for numerical schemes obtained by the "finite difference" approach, *they also apply for finite volume or finite element techniques*

In addition to these properties we must consider *another relevant property of numerical schemes adopted for engineering applications* that can be stated as follows:

while solving by numerical means a conservation equation, care must be taken that no spurious sources or sinks of the conserved quantity will appear even while working with finite space and time increments

In other words, we can afford having an approximate solution of our equations, because of the use of a coarse time or space grid, but we can never afford that the discretization process will not preserve exactly the conserved quantity: this "conservative" character of the numerical schemes is therefore a fundamental requirement

CONVERGENCE, CONSISTENCY AND STABILITY

The numerical methods obtained by any discretization method must possess some basic mathematical features, to be described hereafter

Let us consider *a time-dependent linear partial differential equation*

$$\frac{\partial \psi}{\partial t} = A\psi$$

where A and ψ are a *linear differential operator* and a *function* (in case, the equation may even represent a system of equations and ψ is a vector function). *When discretised in space and time the resulting numerical scheme will have the general form*

$$B_1\,\psi^{n+1} = B_0\,\psi^n$$

where B_1 and B_0 are *finite difference linear operators depending also on the space and time increments and* ψ^n and ψ^{n+1} will be now the *vectors of the values* of ψ at the different space locations and at times t^n and t^{n+1}:

$$B_0 = B_0(\Delta t, \Delta x, \Delta y, \Delta z, ...) \qquad B_1 = B_1(\Delta t, \Delta x, \Delta y, \Delta z, ...).$$

***We must assume that B_1 can be inverted* to allow for time advancement**

$$\psi^{n+1} = B_1^{-1} B_0\,\psi^n = C\,\psi^n$$

where $C = C(\Delta t, \Delta x, \Delta y, \Delta z, ...)$ is the truncated integral operator allowing to obtain ψ^{n+1} from ψ^n.

For simplicity, we assume that there is a link between the space and time increments, such that all of them will vanish when $\Delta t \to 0$

$$\Delta x = g_x(\Delta t) \qquad \Delta y = g_y(\Delta t) \qquad \Delta z = g_z(\Delta t)$$

So, we will write

$$C = C(\Delta t, g_x(\Delta t), g_y(\Delta t), g_z(\Delta t)) = C(\Delta t)$$

<u>Convergence</u>

Assuming to be able to solve the algebraic equations without *round-off error* (the one made by the particular machine in representing a limited number of significant figures), the *discretization error* that we make at the *n*-th time level with respect to the exact solution ψ_e^n is given by

$$\delta^n = \psi_e^n - \psi^n$$

The *total error* would also include *round-off*

For the numerical method to be useful in some respect, *we need that the discretization error can be small enough for small increments*

So, we need that

$$\lim_{\Delta t \to 0} \left\| \delta^n \right\| = 0$$

where $\|\circ\|$ is an appropriate *norm*. This is expressed stating that:

A numerical method is said to be "convergent" if the solution of the discretised equation tends to the exact solution of the differential equation as the grid spacing tends to zero

It can be easily seen that the discretization error δ^n is a result of the approximations made in evaluating the differential (and then the integral) operators, i.e. from *truncation* *(i.e. inaccuracy of the difference operator)*, and from *error propagation* from the previous time step.

In fact:

$$\delta^n = \psi_e^n - C(\Delta t)\psi^{n-1} = \psi_e^n \underbrace{-C(\Delta t)\psi_e^{n-1} + C(\Delta t)\psi_e^{n-1}}_{\text{subtracted and added}} - C(\Delta t)\psi^{n-1}$$

and then

$$\delta^n = \underbrace{\psi_e^n - C(\Delta t)\psi_e^{n-1}}_{\substack{\text{error due to truncation in } C(\Delta t) \\ \text{(the operator is not "exact")}}} + \underbrace{C(\Delta t)\delta^{n-1}}_{\substack{\text{propagation of the} \\ \text{error at time } t^{n-1}}}$$

This calls into play *two other important properties*:

- ***consistency*, expressing the extent at which the finite difference operator is a good approximation of the original differential one;**
- ***stability*, defining the conditions to be respected for limiting the propagation of an error existing at the previous time step.**

Consistency

From the relation

$$\psi^{n+1} = C(\Delta t)\psi^n$$

it is easily obtained

$$\frac{\psi^{n+1} - \psi^n}{\Delta t} = \frac{C(\Delta t) - I}{\Delta t}\psi^n$$

where I is the identity operator.

Comparing this expression with

$$\frac{\partial \psi}{\partial t} = A\psi$$

and considering that it is obviously

$$\frac{\psi^{n+1} - \psi^n}{\Delta t} \to \frac{\partial \psi}{\partial t} \quad for\ \Delta t \to 0$$

we also expect that

$$\frac{C(\Delta t) - I}{\Delta t}\psi(t) \to A\psi(t) \quad for\ \Delta t \to 0$$

In summary, we need that the finite difference equation be *consistent* with the differential one:

$$\frac{\psi(t+\Delta t) - \psi(t)}{\Delta t} - \frac{C(\Delta t) - I}{\Delta t}\psi(t) \to \frac{\partial \psi(t)}{\partial t} - A\psi(t) \quad for\ \Delta t \to 0$$

This is expressed saying that

A numerical scheme is said to be "consistent" with the differential problem if the difference equations representing it tend to those of the differential problem as the grid spacing tends to zero

Consistency is therefore *a property of the form* of the numerical scheme.

The difference between the discretised equations and the partial differential equation is referred to as the *"truncation error".*

In particular, if ψ_e is the exact solution of the differential problem, the *local truncation error* is defined as

$$LTE_{n+1} = \frac{\psi_e^{n+1} - \psi_e^n}{\Delta t} - \frac{C(\Delta t) - I}{\Delta t}\psi_e^n - \underbrace{\left(\frac{\partial \psi_e}{\partial t} - A\psi_e\right)}_{=0} = \frac{\psi_e^{n+1} - C(\Delta t)\psi_e^n}{\Delta t}$$

i.e., it is obtained by applying the numerical scheme to the exact solution ψ_e.

By developing a by *a Taylor series expansion* the difference equations *it is possible to express the truncation error as a function of powers of increments*

<u>Example:</u> Let us approximate the equation

$$\frac{\partial \psi}{\partial t} - \frac{\partial^2 \psi}{\partial x^2} = 0$$

by the finite difference scheme (see below)

$$\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} - \frac{\psi_{i+1}^n - 2\psi_i^n + \psi_{i-1}^n}{\Delta x^2} = 0$$

where ψ_i^n *means* $\psi\left(x_i, t^n\right)$**. Considering that:**

$$\psi_i^{n+1} = \psi_i^n + \left.\frac{\partial \psi}{\partial t}\right|_i^n \Delta t + \left.\frac{\partial^2 \psi}{\partial t^2}\right|_i^n \frac{(\Delta t)^2}{2} + \left.\frac{\partial^3 \psi}{\partial t^3}\right|_i^n \frac{(\Delta t)^3}{6} + \left.\frac{\partial^4 \psi}{\partial t^4}\right|_i^n \frac{(\Delta t)^4}{24} + \ldots$$

$$\psi_{i\pm1}^n = \psi_i^n \pm \left.\frac{\partial \psi}{\partial x}\right|_i^n \Delta x + \left.\frac{\partial^2 \psi}{\partial x^2}\right|_i^n \frac{(\Delta x)^2}{2} \pm \left.\frac{\partial^3 \psi}{\partial x^3}\right|_i^n \frac{(\Delta x)^3}{6} + \left.\frac{\partial^4 \psi}{\partial x^4}\right|_i^n \frac{(\Delta x)^4}{24} + \ldots$$

it is

$$\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} = \left.\frac{\partial \psi}{\partial t}\right|_i^n + \left.\frac{\partial^2 \psi}{\partial t^2}\right|_i^n \frac{\Delta t}{2} + \left.\frac{\partial^3 \psi}{\partial t^3}\right|_i^n \frac{(\Delta t)^2}{6} + \left.\frac{\partial^4 \psi}{\partial t^4}\right|_i^n \frac{(\Delta t)^3}{24} + \ldots$$

$$\frac{\psi_{i+1}^n - 2\psi_i^n + \psi_{i-1}^n}{\Delta x^2} = \left.\frac{\partial^2 \psi}{\partial x^2}\right|_i^n + \left.\frac{\partial^4 \psi}{\partial x^4}\right|_i^n \frac{(\Delta x)^2}{12} + \ldots$$

and then, substituting in the difference equations, it is

$$\left.\frac{\partial \psi}{\partial t}\right|_i^n - \left.\frac{\partial^2 \psi}{\partial x^2}\right|_i^n + \left.\frac{\partial^2 \psi}{\partial t^2}\right|_i^n \frac{\Delta t}{2} - \left.\frac{\partial^4 \psi}{\partial x^4}\right|_i^n \frac{(\Delta x)^2}{12} + \ldots = 0$$

or

$$\left.\frac{\partial \psi}{\partial t}\right|_i^n - \left.\frac{\partial^2 \psi}{\partial x^2}\right|_i^n = O(\Delta t) + O\left(\Delta x^2\right)$$

It can be noted that:

- ***the scheme is consistent*, since *truncation error tends to zero with refining the space and time grid***
- **the *truncation error is first order* in Δt and *second order* in Δx**
- **because of the presence o truncation error, when using finite increments *the actually solved equation is different from the original one*: a *modified equation* is actually solved including higher order derivatives**

Stability

In short, it can be stated that:

A numerical scheme is said "stable" if it does not amplify the errors appearing during the numerical solution process

Since it is

$$\delta^1 = \psi_e^1 - C(\Delta t)\psi_e^0 + C(\Delta t)\psi_e^0 - C(\Delta t)\psi^0 = \Delta t\, LTE_1 + C(\Delta t)\delta^0$$

$$\delta^2 = \Delta t\, LTE_2 + C(\Delta t)\delta^1 = \Delta t\, LTE_2 + \Delta t\, C(\Delta t) LTE_1 + C^2(\Delta t)\delta^0$$

.....

$$\delta^n = \Delta t \sum_{i=1}^{n} C^{n-i}(\Delta t) LTE_i + C^n(\Delta t)\delta^0$$

it can be noted that "stability" is related to the "boundedness" of the difference operators $C^n(\Delta t)$ in the functional domain in which they operate, i.e. to *their property to damp (and not amplify) these functions* and hence the errors.

In fact, it is noted that *even if we assume no error on the initial data*, i.e. $\delta^0 = 0$, *we necessarily have to take into account that the local truncation error at each step* will appear: this should be damped to guarantee a limited discretization error

$$\delta^n = \Delta t \sum_{i=1}^{n} C^{n-i}(\Delta t)\, LTE_i \qquad if\ \ \delta^0 = 0$$

In fact, *local truncation error at each step will be always obtained because of the use of finite increments* (we cannot really avoid it!)

***Different techniques are available to check stability*. A well known one is *the von Neumann stability criterion* in which a perturbation is given to the values of the variable at the previous time-step and it is assumed that it propagates in space and time as:**

$$\delta(x,t) = \delta_i^n e^{\alpha\left(t-t^n\right)} e^{i\beta(x-x_i)} \qquad ([2])\ ([3])\ \textbf{with } \alpha \in \mathbf{C},\ \beta \in \mathbf{R}$$

It can be shown that the perturbed, ψ, and the non perturbed solutions, $\tilde{\psi}_{np}$, must satisfy the same equation. In fact:

$$\tilde{\psi}_{np}(x,t+\Delta t) = C(\Delta t,\Delta x)\tilde{\psi}_{np}(x,t)$$

and

$$\psi(x,t+\Delta t) = C(\Delta t,\Delta x)\psi(x,t)$$

$$or \qquad \tilde{\psi}_{np}(x,t+\Delta t) + \delta(x,t+\Delta t) = C(\Delta t,\Delta x)\left[\tilde{\psi}_{np}(x,t) + \delta(x,t)\right]$$

since it is $\psi(x,t) = \tilde{\psi}_{np}(x,t) + \delta(x,t)$. As a consequence the same equation is satisfied by the perturbation

$$\delta(x,t+\Delta t) = C(\Delta t,\Delta x)\delta(x,t)$$

The quantity

$$G(\Delta t,\Delta x) = \frac{\delta(x,t+\Delta t)}{\delta(x,t)}$$

being a ratio of complex numbers, is said *amplification factor* and its magnitude allows discussing stability.

In particular, *the criterion for stability is*

$$\boxed{\left|G(\Delta t,\Delta x)\right| = \left|e^{\alpha\Delta t}\right| \le 1} \qquad \textbf{\textit{(von Neumann condition)}}$$

and requires *to study the real part of α for arbitrary $\beta\Delta x$*.

The above condition applies *when the exact solution does not increase with time*; whenever it is not so, it is necessary to impose the criterion

$$\boxed{\left|G(\Delta t,\Delta x)\right| \le 1 + K\,\Delta t} \qquad \textbf{\textit{(von Neumann necessary condition)}}$$

([2]) Consider that, though here we are using for the error propagated the same notation δ as for the discretisation error, the latter represents a broader concept, including also truncation error.

([3]) Note that β has the role of a "wave number" of the perturbation. Considering that perturbations will generally contain a wide variety of wave numbers, demonstrating stability means demonstrating that for any wave number the perturbation will not grow.

Example: **The dimensionless heat diffusion equation, again represented in "explicit" (see later on) and dimensionless form is:**

$$\frac{\partial \psi}{\partial t} - \frac{\partial^2 \psi}{\partial x^2} = 0 \qquad \rightarrow \qquad \frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} - \frac{\psi_{i+1}^n - 2\psi_i^n + \psi_{i-1}^n}{\Delta x^2} = 0$$

It is:

$$\frac{\delta_i^{n+1} - \delta_i^n}{\Delta t} - \frac{\delta_{i+1}^n - 2\delta_i^n + \delta_{i-1}^n}{\Delta x^2} = 0$$

with

$$\delta_i^{n+1} = \delta_i^n e^{\alpha \Delta t} \qquad \delta_{i-1}^n = \delta_i^n e^{-i\beta \Delta x} \qquad \delta_{i+1}^n = \delta_i^n e^{i\beta \Delta x}$$

Therefore

$$\frac{e^{\alpha \Delta t} - 1}{\Delta t} - \frac{e^{i\beta \Delta x} - 2 + e^{-i\beta \Delta x}}{\Delta x^2} = 0 \rightarrow e^{\alpha \Delta t} = 1 + \frac{\Delta t}{\Delta x^2}\left[\left(e^{i\beta \Delta x} + e^{-i\beta \Delta x}\right) - 2\right]$$

$$|G| = \left|e^{\alpha \Delta t}\right| = \left|1 + \frac{2\Delta t}{\Delta x^2}\left[\cos(\beta \Delta x) - 1\right]\right| \leq 1 \Rightarrow \frac{2\Delta t}{\Delta x^2} \leq 1$$

This means that a *conditional stability* is found, where *the time step must be limited by the relation*:

$$\Delta t \leq \frac{\Delta x^2}{2}$$

which can be *a very severe limitation* when the spatial increment is small!

When referring to the heat equation in dimensional form:

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0 \qquad \rightarrow \qquad \frac{T_i^{n+1} - T_i^n}{\Delta t} - \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} = 0$$

the criterion assumes the form

$$\frac{\alpha \Delta t}{\Delta x^2} \leq \frac{1}{2}$$

By similar developments it can be shown that the "implicit" formulation (see below)

$$\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} - \frac{\psi_{i+1}^{n+1} - 2\psi_i^{n+1} + \psi_{i-1}^{n+1}}{\Delta x^2} = 0$$

is *unconditionally stable*, as it is for many "implicit" numerical schemes.

In fact, it is:

$$\frac{\delta_i^{n+1}-\delta_i^n}{\Delta t}-\frac{\delta_{i+1}^{n+1}-2\delta_i^{n+1}+\delta_{i-1}^{n+1}}{\Delta x^2}=0$$

where

$$\delta_i^n=\delta_i^{n+1}e^{-\alpha\Delta t} \qquad \delta_{i-1}^{n+1}=\delta_i^{n+1}e^{-i\beta\Delta x} \qquad \delta_{i+1}^{n+1}=\delta_i^{n+1}e^{i\beta\Delta x}$$

So

$$\frac{1-e^{-\alpha\Delta t}}{\Delta t}-\frac{e^{i\beta\Delta x}-2+e^{-i\beta\Delta x}}{\Delta x^2}=0\rightarrow e^{-\alpha\Delta t}=1+\frac{\Delta t}{\Delta x^2}\left[2-\left(e^{i\beta\Delta x}+e^{-i\beta\Delta x}\right)\right]$$

$$|G|=\left|e^{\alpha\Delta t}\right|=\left|\left\{1+\frac{2\Delta t}{\Delta x^2}\left[1-\cos\left(\beta\Delta x\right)\right]\right\}^{-1}\right|\leq 1 \; \textit{that is always true}$$

Lax Equivalence Theorem

Given a properly posed linear initial value problem and a finite difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence

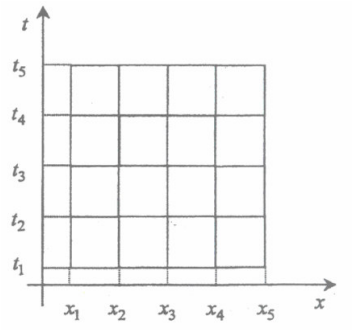
The demonstration, that we omit, follows from the above formulation adopted for the discretization error and holds for linear problems.

Consistency and Stability are therefore the properties to be possessed by a numerical scheme to achieve Convergence.

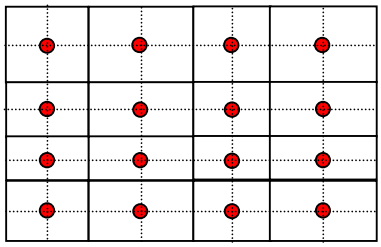
Domain discretization

The space and time domain must be *discretised* by introducing appropriate *grids* (a "mesh") whose characteristics may vary depending on the discretization scheme.

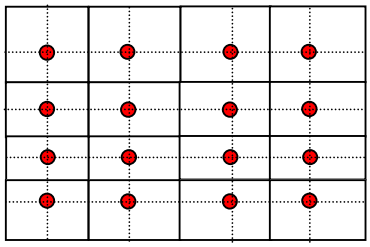
A simple Cartesian grid as the one described below can be used for time and space discretization of 1D problems.



Centered nodes or centered faces can be used in the case of 2D or 3D finite volumes according to accuracy constraints

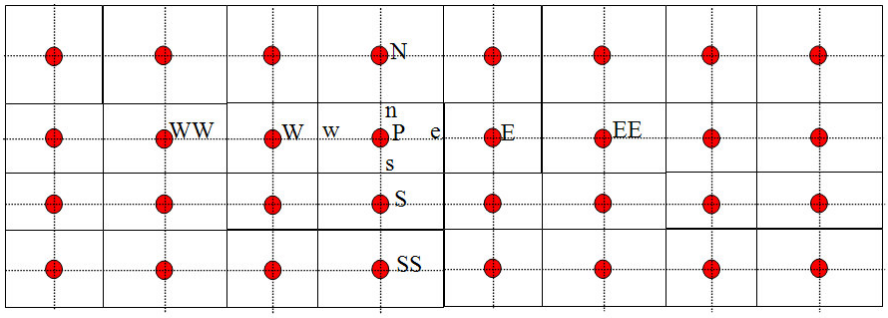


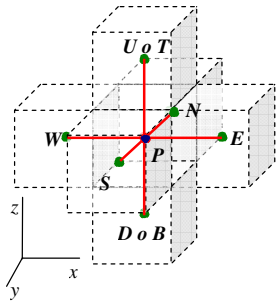
Centered nodes



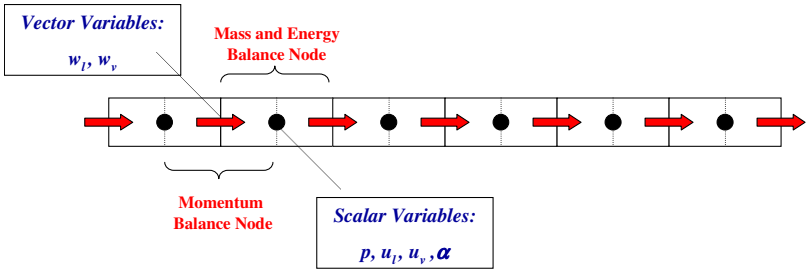
Centered faces

A *typical nomenclature* is used in 2D and 3D for defining a node and its neighbouring ones

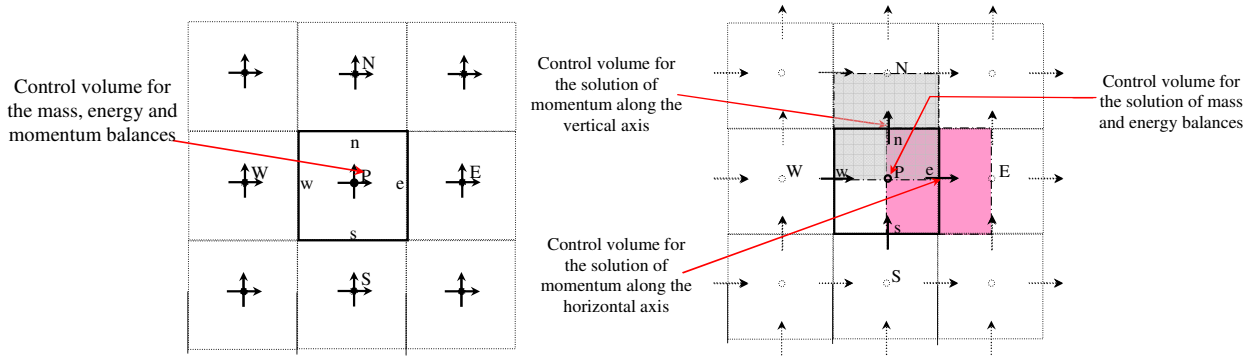




The use of *"control volumes"* and *"junctions"* is also *typical of system codes for single and two-phase flow applications*. Often, *the nodes are "staggered"* to solve mass and energy equations in different control volumes:

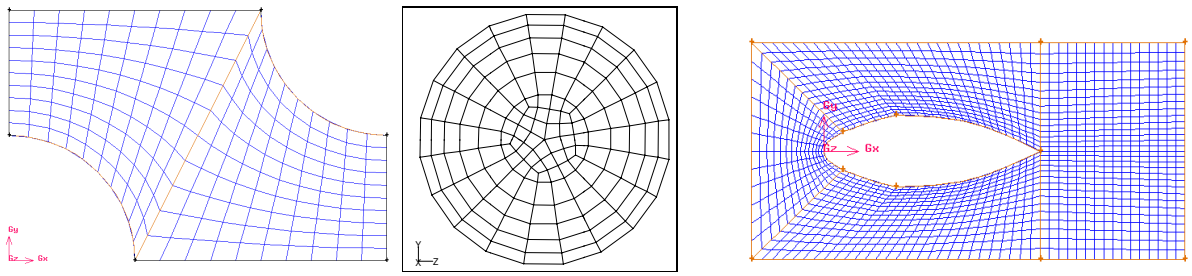


***Collocated* or *staggered grids* are also used in CFD. By the latter approach a more direct use of velocities evaluated at the interfaces is made in mass and energy balance equations**

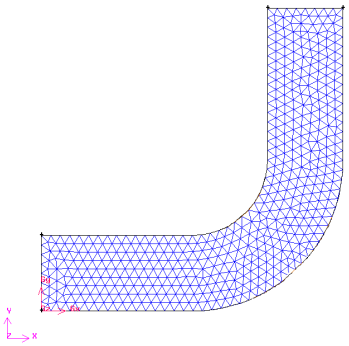


More complex grids can be generated *to better fit bodies*. *Structured grids* are those in which *different families of curves are present and the curves of a family do not intersect each other, while they do intersect the curves of the other families*. *Unstructured grids* do not respect this definition.

In structured grids, each node can be identified by the indices of the curves of the intersecting families, while it is not the case for unstructured grids

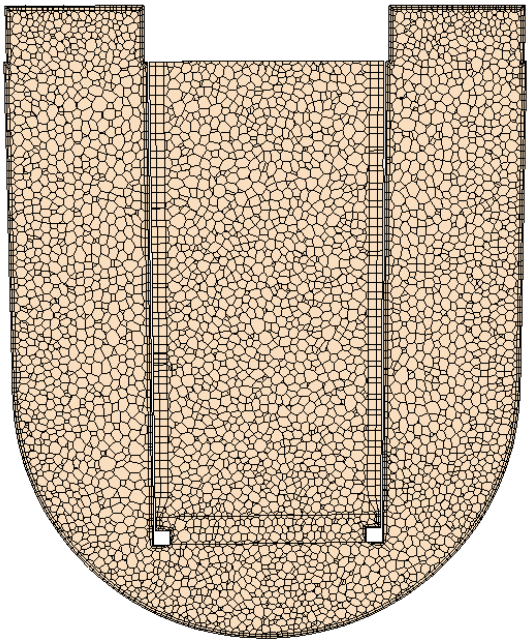


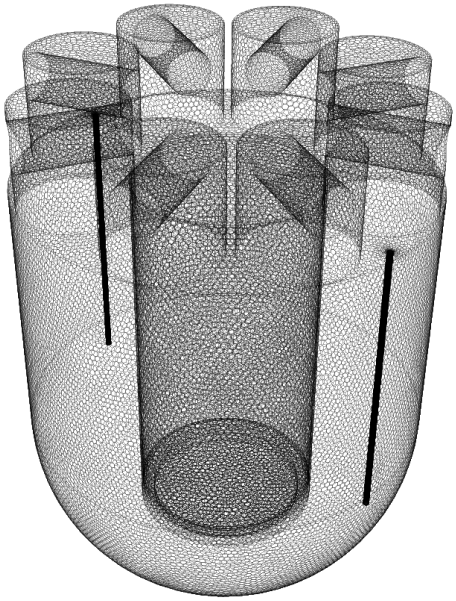
Structured grids of types "H", "O" and "C" and "H"



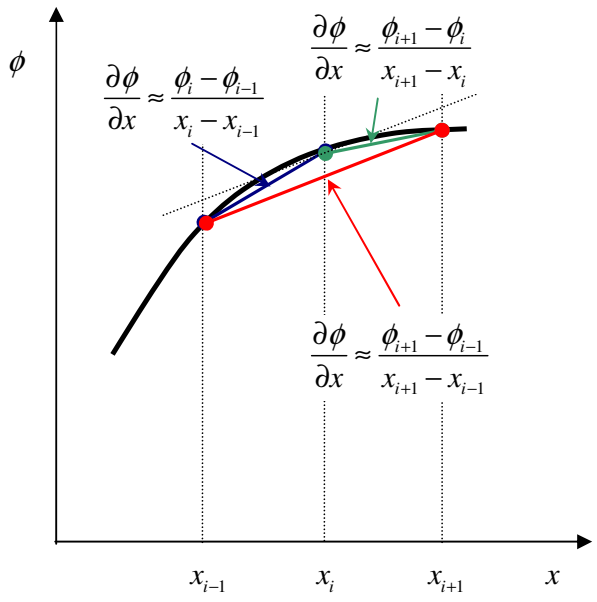
Example of unstructured grid

Very complex grids, made by *tetrahedral* or *polyhedral* finite volumes or finite elements, can be adopted for complex geometries. Sometimes, refinements close to the walls are needed to better represent the structure of turbulent boundary layers.





FINITE DIFFERNCES, FINITE VOLUMES AND FINITE ELEMENTS



Finite Differences

In substituting first derivatives with finite difference expressions different choices can be adopted (in the following, we assume $\phi_i = \phi(x_i)$ and so on)

- ***backward differences***

$$\left(\frac{\partial\phi}{\partial x}\right)_{x_i} \approx \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}$$

- ***forward differences***

$$\left(\frac{\partial\phi}{\partial x}\right)_{x_i} \approx \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i}$$

- ***centered differences***

$$\left(\frac{\partial\phi}{\partial x}\right)_{x_i} \approx \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}}$$

In a more systematic way, additional and more complex expressions can be obtained making use of Taylor expansion or differentiating polynomial interpolation curves. It is interesting to note that the expansion in Taylor series around x_i leads to

$$\phi_{i\pm1} = \phi_i + \left(\frac{\partial\phi}{\partial x}\right)_i (x_{i\pm1} - x_i) + \left(\frac{\partial^2\phi}{\partial x^2}\right)_i \frac{(x_{i\pm1} - x_i)^2}{2!} + \left(\frac{\partial^3\phi}{\partial x^3}\right)_i \frac{(x_{i\pm1} - x_i)^3}{3!} + \ldots$$

and so

$$\phi_{i-1} = \phi_i - \left(\frac{\partial\phi}{\partial x}\right)_i (x_i - x_{i-1}) + \left(\frac{\partial^2\phi}{\partial x^2}\right)_i \frac{(x_i - x_{i-1})^2}{2!} - \left(\frac{\partial^3\phi}{\partial x^3}\right)_i \frac{(x_i - x_{i-1})^3}{3!} + \ldots$$

$$\phi_{i+1} = \phi_i + \left(\frac{\partial\phi}{\partial x}\right)_i (x_{i+1} - x_i) + \left(\frac{\partial^2\phi}{\partial x^2}\right)_i \frac{(x_{i+1} - x_i)^2}{2!} + \left(\frac{\partial^3\phi}{\partial x^3}\right)_i \frac{(x_{i+1} - x_i)^3}{3!} + \ldots$$

It is therefore:

$$\frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}=\left(\frac{\partial\phi}{\partial x}\right)_i-\left(\frac{\partial^2\phi}{\partial x^2}\right)_i\frac{\left(x_i-x_{i-1}\right)}{2!}+\left(\frac{\partial^3\phi}{\partial x^3}\right)_i\frac{\left(x_i-x_{i-1}\right)^2}{3!}+\ldots$$

$$\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}=\left(\frac{\partial\phi}{\partial x}\right)_i+\left(\frac{\partial^2\phi}{\partial x^2}\right)_i\frac{\left(x_{i+1}-x_i\right)}{2!}+\left(\frac{\partial^3\phi}{\partial x^3}\right)_i\frac{\left(x_{i+1}-x_i\right)^2}{3!}+\ldots$$

or

$$\left(\frac{\partial\phi}{\partial x}\right)_i=\frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}+\left(\frac{\partial^2\phi}{\partial x^2}\right)_i\frac{\left(x_i-x_{i-1}\right)}{2!}-\left(\frac{\partial^3\phi}{\partial x^3}\right)_i\frac{\left(x_i-x_{i-1}\right)^2}{3!}+\ldots$$

$$\left(\frac{\partial\phi}{\partial x}\right)_i=\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}-\left(\frac{\partial^2\phi}{\partial x^2}\right)_i\frac{\left(x_{i+1}-x_i\right)}{2!}-\left(\frac{\partial^3\phi}{\partial x^3}\right)_i\frac{\left(x_{i+1}-x_i\right)^2}{3!}+\ldots$$

So, these expressions obtained by forward or backward differences *introduce higher order terms* proportional to x_i-x_{i-1} or $x_{i+1}-x_i$: it is said that they are *first order accurate in* Δx, i.e. the order of their truncation error is the first in the spatial increment.

On the other hand, for the centered difference expression it is:

$$\frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}}=\left(\frac{\partial\phi}{\partial x}\right)_i+\left(\frac{\partial^2\phi}{\partial x^2}\right)_i\frac{\left(x_{i+1}-x_i\right)^2-\left(x_i-x_{i-1}\right)^2}{2!\left(x_{i+1}-x_{i-1}\right)}+\left(\frac{\partial^3\phi}{\partial x^3}\right)_i\frac{\left(x_{i+1}-x_i\right)^3+\left(x_i-x_{i-1}\right)^3}{3!\left(x_{i+1}-x_{i-1}\right)}+\ldots$$

or

$$\left(\frac{\partial\phi}{\partial x}\right)_i=\frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}}-\left(\frac{\partial^2\phi}{\partial x^2}\right)_i\frac{\left(x_{i+1}-x_i\right)^2-\left(x_i-x_{i-1}\right)^2}{2!\left(x_{i+1}-x_{i-1}\right)}-\left(\frac{\partial^3\phi}{\partial x^3}\right)_i\frac{\left(x_{i+1}-x_i\right)^3+\left(x_i-x_{i-1}\right)^3}{3!\left(x_{i+1}-x_{i-1}\right)}+\ldots$$

It can be noted that, *in the case of uniform discretization*, it is:

$$\left(\frac{\partial\phi}{\partial x}\right)_i=\frac{\phi_{i+1}-\phi_{i-1}}{2\Delta x}-\left(\frac{\partial^3\phi}{\partial x^3}\right)_i\frac{\Delta x^2}{3!}+\ldots$$

showing that *the expression with centered differences with uniform grid is "second order" accurate in* Δx*;* this means a greater accuracy with respect to first order, since the approximate expression tends to the derivative "*faster*" when $\Delta x\to 0$ (i.e., with Δx^2).

For *higher order derivatives it is possible to adopt the numerical differentiation of finite difference expressions*. For instance:

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_i \approx \frac{\left(\frac{\partial\phi}{\partial x}\right)_{i+1/2} - \left(\frac{\partial\phi}{\partial x}\right)_{i-1/2}}{\frac{1}{2}\left(x_{i+1} - x_{i-1}\right)} \approx \frac{\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i} - \frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}}{\frac{1}{2}\left(x_{i+1}-x_{i-1}\right)} = \frac{\left(\phi_{i+1}-\phi_i\right)\Delta x_i - \left(\phi_i-\phi_{i-1}\right)\Delta x_{i+1}}{\frac{1}{2}\left(\Delta x_{i+1}+\Delta x_i\right)\Delta x_i \Delta x_{i+1}}$$

$$= \frac{\phi_{i+1}\Delta x_i + \phi_{i-1}\Delta x_{i+1} - \phi_i\left(\Delta x_i + \Delta x_{i+1}\right)}{\frac{1}{2}\left(\Delta x_{i+1}+\Delta x_i\right)\Delta x_i \Delta x_{i+1}}$$

For uniform discretization, it is:

$$\boxed{\left(\frac{\partial^2\phi}{\partial x^2}\right)_i \approx \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\left(\Delta x\right)^2}}$$

That is a well known expression, already used above, for discretizing the diffusion equation

$$\left(\frac{\partial^2\phi}{\partial x^2}\right)_i = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\left(\Delta x\right)^2} - \left(\frac{\partial^4\phi}{\partial x^4}\right)_i \frac{\left(\Delta x\right)^2}{12} + \ldots$$

Sometimes, for diffusion terms, *it is more convenient to differentiate directly the fluxes to account for the change in the diffusion coefficients*

$$\left[\frac{\partial}{\partial x}\left(\Gamma\frac{\partial\phi}{\partial x}\right)\right]_i \approx \frac{\left(\Gamma\frac{\partial\phi}{\partial x}\right)_{i+1/2} - \left(\Gamma\frac{\partial\phi}{\partial x}\right)_{i-1/2}}{\frac{1}{2}\left(x_{i+1}-x_{i-1}\right)} \approx \frac{\Gamma_{i+1/2}\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i} - \Gamma_{i-1/2}\frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}}{\frac{1}{2}\left(x_{i+1}-x_{i-1}\right)}$$

Up to now we implicitly assumed differentiation with respect to a spatial variable. Similar techniques can be adopted the time derivatives of time-varying variables (in the following, ϕ_i^n will indicate $\phi\left(x_i, t^n\right)$).

For instance, a *forward* difference will lead to:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \left.\frac{\partial\phi}{\partial t}\right|_i^n + \left.\frac{\partial^2\phi}{\partial t^2}\right|_i^n \frac{\Delta t}{2} + \left.\frac{\partial^3\phi}{\partial t^3}\right|_i^n \frac{\left(\Delta t\right)^2}{6} + \left.\frac{\partial^4\phi}{\partial t^4}\right|_i^n \frac{\left(\Delta t\right)^3}{24} + \ldots$$

In similarity with what seen for spatial derivatives, it is clear that we can obtain *a greater accuracy with a centered difference expression*

$$\left(\frac{\partial \phi}{\partial t}\right)_i^n \approx \frac{\phi_i^{n+1} - \phi_i^{n-1}}{2\Delta t}$$

obtaining a second order approximation in Δt.

In a more general approach for space and time discretization, we can consider the differential equation

$$\frac{\partial \phi}{\partial t} = L\phi$$

where L is a differential operator containing spatial derivatives and source terms. By spatial discretization we get:

$$\frac{\partial \phi}{\partial t} = L_a\phi$$

where L_a is *a finite difference operator obtained by discretizing* L. We can now proceed to integrate both sides of the equation in time over a finite time step:

$$\phi_i^{n+1} = \phi_i^n + \int_{t^n}^{t^{n+1}} L_a\phi \, dt$$

We can make *different assumptions on the time variation of the integrand function*. In this respect, we have *three classical assumptions*:

- ***explicit method*:** $\phi_i^{n+1} = \phi_i^n + L_a\phi^n \Delta t$
- ***implicit method*:** $\phi_i^{n+1} = \phi_i^n + L_a\phi^{n+1} \Delta t$
- ***Crank-Nicolson method*:** $\phi_i^{n+1} = \phi_i^n + \frac{1}{2}\left[L_a\phi^{n+1} + L_a\phi^n\right]\Delta t$

The latter is more accurate, since *it is similar to a centered differencing* in time. A general formulation for the three methods is:

$$\phi_i^{n+1} = \phi_i^n + \left[\alpha L_a\phi^{n+1} + (1-\alpha) L_a\phi^n\right]\Delta t \qquad 0 \le \alpha \le 1$$

A relevant example: finite difference discretization of the advection equation

It is rather instructive to consider the simple hyperbolic equation

$$\boxed{\frac{\partial T}{\partial t} + w\frac{\partial T}{\partial x} = 0}$$

This equation is relevant for us because:

- ***the advective part of the balance equations represents and important feature* that needs to be carefully discretised;**
- ***when a propagation phenomenon is hyperbolic in nature* (e.g., pressure perturbations), *we always have to take into account the finite speed of propagation of perturbations* (e.g., the *fluid velocity* or the *speed of sound*)**

Two widespread difference schemes for this equation are:

- **the *"upwind explicit"* method**

$$\begin{aligned} &\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_i^n-T_{i-1}^n}{\Delta x}=0, \qquad w\geq 0 \\ &\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_{i+1}^n-T_i^n}{\Delta x}=0, \qquad w<0 \end{aligned}$$

- **the *"upwind implicit"* method**

$$\begin{aligned} &\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_i^{n+1}-T_{i-1}^{n+1}}{\Delta x}=0, \quad w\geq 0 \\ &\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_{i+1}^{n+1}-T_i^{n+1}}{\Delta x}=0, \quad w<0 \end{aligned}$$

It can be shown that, in the limit of small increments, these two methods formally tend to the original partial differential equation:

$$\begin{aligned} &\lim_{\substack{\Delta t\to 0\\ \Delta x\to 0}}\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_i^n-T_{i-1}^n}{\Delta x}=\left.\frac{\partial T}{\partial t}\right|_i^n+w\left.\frac{\partial T}{\partial x}\right|_i^n \\ &\lim_{\substack{\Delta t\to 0\\ \Delta x\to 0}}\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_i^{n+1}-T_{i-1}^{n+1}}{\Delta x}=\left.\frac{\partial T}{\partial t}\right|_i^n+w\left.\frac{\partial T}{\partial x}\right|_i^n \end{aligned}$$

***So consistency is verified*. The application of the *von Neumann stability criterion* (see above) shows that the explicit upwind scheme is *conditionally stable* and, in particular, it is stable provided that**

$$Courant\ number=\frac{w\Delta t}{\Delta x}\leq 1$$

(Courant-Friederichs-Lewy condition)

while the upwind implicit one is *unconditionally stable*.

The latter represents an "advantage" of the implicit methods, since there is no need to select particular couples of Δt and Δx to assure stability. It will be seen that *this advantage has a price and some drawbacks*.

Demonstrations about stability:

- ***Upwind explicit scheme***

  Given the scheme

$$\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_i^n-T_{i-1}^n}{\Delta x}=0$$

  the error must satisfy the condition:

$$\frac{\delta_i^{n+1}-\delta_i^n}{\Delta t}+w\frac{\delta_i^n-\delta_{i-1}^n}{\Delta x}=0$$

  where we put

$$\delta_i^{n+1}=\delta_i^n e^{\alpha\Delta t} \qquad \delta_{i-1}^n=\delta_i^n e^{-i\beta\Delta x}$$

  Then, it is

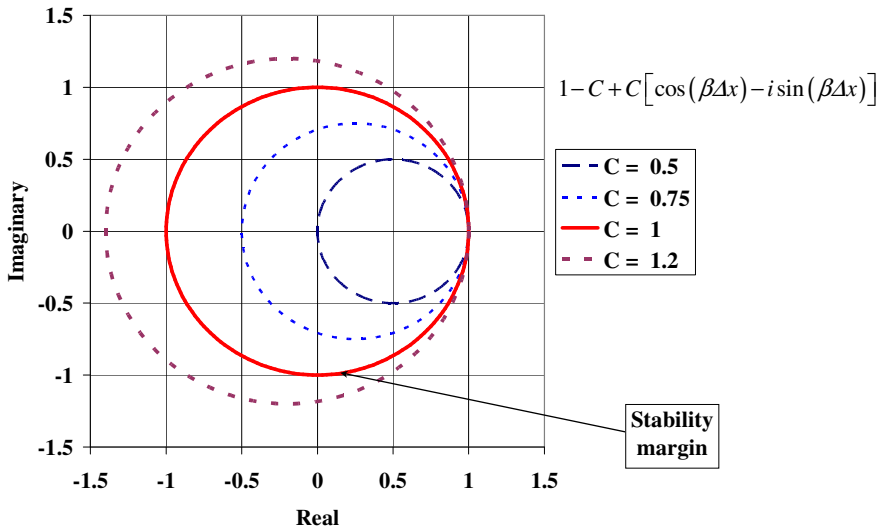
$$\frac{\delta_i^n e^{\alpha\Delta t}-\delta_i^n}{\Delta t}+w\frac{\delta_i^n-\delta_i^n e^{-i\beta\Delta x}}{\Delta x}=0 \quad\Rightarrow\quad \frac{e^{\alpha\Delta t}-1}{\Delta t}+w\frac{1-e^{-i\beta\Delta x}}{\Delta x}=0$$

$$\Rightarrow\quad e^{\alpha\Delta t}=1-\frac{w\Delta t}{\Delta x}\left(1-e^{-i\beta\Delta x}\right) \quad\Rightarrow\quad e^{\alpha\Delta t}=1-C\left(1-e^{-i\beta\Delta x}\right)$$

  where we have put $C=Courant\ number=\frac{w\Delta t}{\Delta x}$ **; the stability criterion is:**

$$|G|=\left|e^{\alpha\Delta t}\right|=\left|1-C\left[1-\cos(\beta\Delta x)+i\sin(\beta\Delta x)\right]\right|$$
$$=\left|1-C+C\left[\cos(\beta\Delta x)-i\sin(\beta\Delta x)\right]\right|\le 1$$

This condition implies that *the Courant number must be less or equal to unity*, as shown in the figure representing the obtained complex number at varying values of the Courant number



- ***Upwind implicit scheme***

  Given the scheme

$$\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_i^{n+1}-T_{i-1}^{n+1}}{\Delta x}=0$$

  the error must satisfy the condition:

$$\frac{\delta_i^{n+1}-\delta_i^n}{\Delta t}+w\frac{\delta_i^{n+1}-\delta_{i-1}^{n+1}}{\Delta x}=0$$

  In this case, it is more convenient to put

$$\delta_i^n=\delta_i^{n+1}e^{-\alpha\Delta t}\qquad\qquad \delta_{i-1}^{n+1}=\delta_i^{n+1}e^{-i\beta\Delta x}$$

  Then, it is

$$\frac{\delta_i^{n+1}-\delta_i^{n+1}e^{-\alpha\Delta t}}{\Delta t}+w\frac{\delta_i^{n+1}-\delta_i^{n+1}e^{-i\beta\Delta x}}{\Delta x}=0 \quad\Rightarrow\quad \frac{1-e^{-\alpha\Delta t}}{\Delta t}+w\frac{1-e^{-i\beta\Delta x}}{\Delta x}=0$$

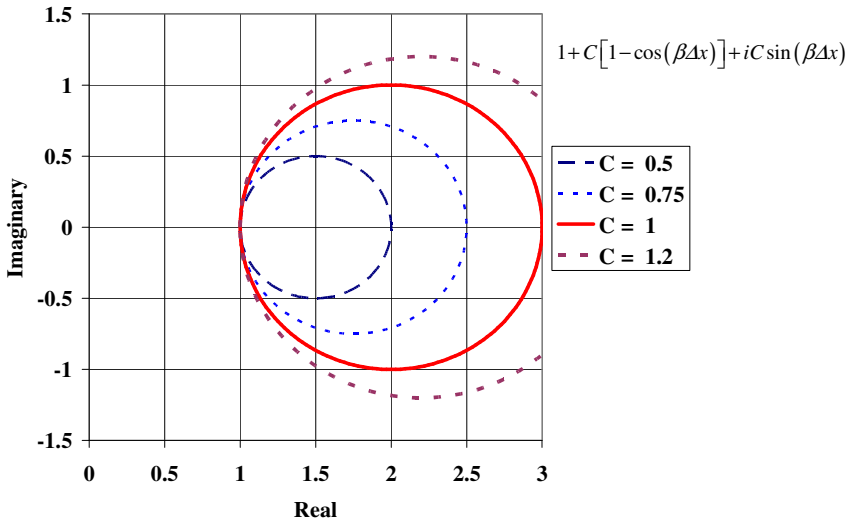
$$\Rightarrow\quad e^{-\alpha\Delta t}=1+\frac{w\Delta t}{\Delta x}\left(1-e^{-i\beta\Delta x}\right)\quad\Rightarrow\quad e^{-\alpha\Delta t}=1+C\left(1-e^{-i\beta\Delta x}\right)$$

$$\Rightarrow\quad e^{\alpha\Delta t}=\frac{1}{1+C\left(1-e^{-i\beta\Delta x}\right)}$$

  In this case, being

$$|G|=\left|e^{\alpha\Delta t}\right|=\left|\frac{1}{1+C\left[1-\cos(\beta\Delta x)\right]+iC\sin(\beta\Delta x)}\right|\le 1$$

  it is sufficient to demonstrate that the complex number at the denominator has a magnitude greater or equal to unity for any value of the Courant number **as shown in the figure below**



Despite of its conditional stability, it must be noted that *an explicit formulation is rather simple since all the values of the unknowns at the new time step are immediately calculated on the basis of old values*

$$T_i^{n+1} = \left(1 - \frac{w\Delta t}{\Delta x}\right) T_i^n + \frac{w\Delta t}{\Delta x} T_{i-1}^n, \qquad w \geq 0$$

An implicit formulation, instead, involves in general the solution of coupled equations: this is the mentioned *"price"*

$$T_i^{n+1}\left(1 + \frac{w\Delta t}{\Delta x}\right) - \frac{w\Delta t}{\Delta x} T_{i-1}^{n+1} = T_i^n, \qquad w \geq 0$$

As a drawback for its simplicity, the explicit methods are limited in the fact that they can propagate only information known at the previous time step. In fact, the limitation on the Courant number implies that

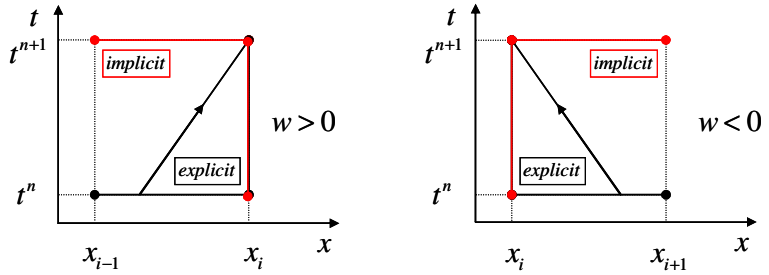
a node of length Δx cannot be swept completely during a time step since in that case there would be no information available on the upwind value of the scalar to be advected

$$THEREFORE\ IT\ MUST\ BE: \quad \Delta t \leq \Delta x / w = node\ sweeping\ time$$

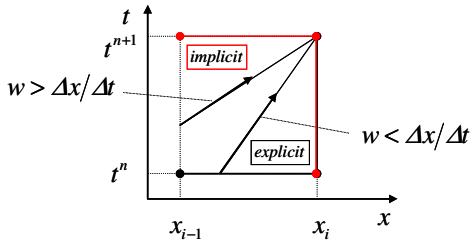
This is not necessary in the case of implicit scheme, as the updated values of the scalar *are evaluated simultaneously everywhere*

Several formulations exist to deal with convective terms in balance equations, which are even more accurate than first order upwind. *However, "upwind differencing" represents a simple interesting choice since it basically reflects the transport of information in the original hyperbolic advection equation*

The upwind choice, in fact, *approximates the direction of the characteristic lines*, i.e., of the lines along which the perturbations of the advected scalar are propagated in space and time



Whether the explicit or the implicit scheme should be used, depends on how fast is the phenomenon to be simulated and which is a convenient space and time grid

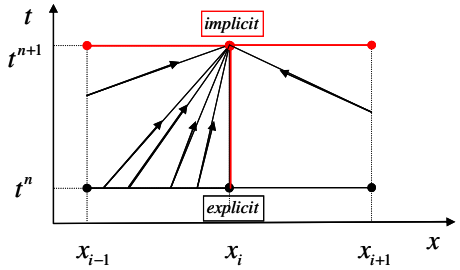


In particular:

- ***for very fast phenomena,* for which it is not needed to have detailed information on short time windows, *implicit discretization* should be used to avoid severe Courant limitations**
- ***for slower phenomena* or detailed time analysis, the explicit scheme should be chosen**

In complex phenomena, like two-phase flow, there are simultaneous perturbations characterised by *different speeds of propagation of information*:

- ***pressure perturbations: propagated at the speed of sound***
- ***thermal coupling between the phases: a very fast phenomenon***
- ***scalar (e.g., temperature, concentration, etc.) advection: propagated with the velocities of the mixture or of the phases***
- ***void propagation: slightly different speed as the mixture fluid***



In such a "stiff" situation, two main alternatives are available:

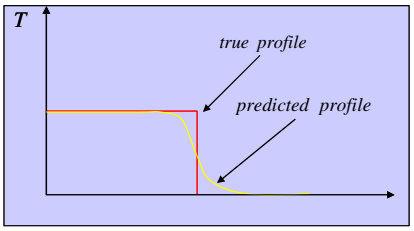
- ***fully implicit approach (e.g., CATHARE)***
- ***split phenomena and use a partially implicit numerical scheme (e.g., RELAP5), explicit for the slower phenomena and implicit for the faster ones***

Concerning accuracy, it can be shown that the truncation error in implicit methods is larger than in explicit ones. In fact, the related *modified equation* has *a larger "numerical diffusion"* coefficient: *this is the mentioned "drawback"*

$$\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_i^n-T_{i-1}^n}{\Delta x}=0 \quad \Rightarrow \quad \frac{\partial T}{\partial t}+w\frac{\partial T}{\partial x}=\left(1-\frac{w\Delta t}{\Delta x}\right)\frac{w\Delta x}{2}\frac{\partial^2 T}{\partial x^2}+HOT$$

$$\frac{T_i^{n+1}-T_i^n}{\Delta t}+w\frac{T_i^{n+1}-T_{i-1}^{n+1}}{\Delta x}=0 \quad \Rightarrow \quad \frac{\partial T}{\partial t}+w\frac{\partial T}{\partial x}=\left(1+\frac{w\Delta t}{\Delta x}\right)\frac{w\Delta x}{2}\frac{\partial^2 T}{\partial x^2}+HOT$$

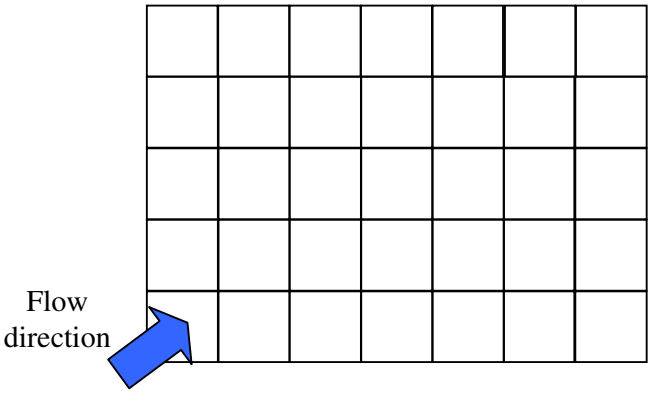
Numerical diffusion is responsible in this case for the introduction of *a sort of fictitious axial heat conduction* smearing out sharp fronts (this phenomenon is called "dissipation")



The *odd numbered higher order derivatives* appearing in the higher order terms (HOT) of truncation error introduce *"dispersive" effects*, i.e. a splitting of the propagation velocity of the different harmonic components of a perturbation

Dissipation **(from even order derivatives) and** ***dispersion*** **(from odd order derivatives) build up to generate** ***the whole effect of truncation error*** **that is referred to with the name of** ***"numerical diffusion"***

It is mentioned that a similar effect occurs also in multidimensional steady-state calculations when the flow is not aligned with the grid *("cross wind diffusion")*



Finite Volume Method

The computational domain is subdivided into *control volumes* (CV = control volumes) where the equations are solved in integral form

$$\underbrace{\frac{d}{dt}\int_V \rho\phi\, dV}_{\substack{\text{Rate of change}\\ \text{of } \Phi \text{ in } V}} = \underbrace{-\int_S \rho\phi\, \mathbf{w}\cdot\mathbf{n}\, dS}_{\substack{\text{Flux of } \Phi \text{ out of } S\\ \text{due to fluid motion}\\ \text{(advection or convection)}}} + \underbrace{\int_S \Gamma_\phi \nabla\phi\cdot\mathbf{n}\, dS}_{\substack{\text{Flux of } \Phi \text{ out of } S\\ \text{due to molecular motion}\\ \text{(diffusion)}}} + \underbrace{\int_V \rho S_\phi\, dV}_{\substack{\text{Volumetric}\\ \text{source of } \Phi}}$$

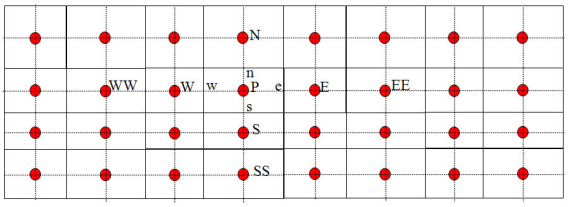
Different, even very complicated, grids can be used in staggered or collocated arrangements

The *surface integrals* appearing in the balance equations are written as the summation of the integrals on the different surfaces

$$\int_S \psi\, dS = \sum_j \int_{S_j} \psi\, dS$$

where ψ is here the generic *"flux"* term.

The evaluation of these integrals is anyway conditioned by *the availability of a value of ψ at the interface*; for instance, in 2D it is



$$\int_{S_e} \psi\, dS \approx \psi_e\, S_e \qquad \int_{S_w} \psi\, dS \approx \psi_w\, S_w \quad \textbf{ecc.}$$

e.g., defining a value of the integrand function in the middle of the interface. More accurate choices are available.

Volume integrals*, instead, are simply evaluated as *the product of the nodal value* (taken as the average in the node) *by the volume

$$\int_V q\, dV \approx q_P\, V$$

where q is the general volumetric term. Also in this case, more accurate choices may be adopted.

In order to determine the values of the integrand functions not immediately available in the calculation at the interfaces, it is necessary to introduce interpolation methods.

This problem is typical, for instance, of the *scalar values* (e.g., densities, enthalpies) at the interfaces. Different possibilities are available for the variable ϕ in the advection term $\rho\phi\mathbf{w}\cdot\mathbf{n}$, assuming that the other quantities are known:

- ***"upwind differencing scheme (UDS)":***

$$\phi_e = \begin{cases} \phi_P, & if \quad (\mathbf{w}\cdot\mathbf{n}_x)_e \geq 0 \\ \phi_E, & if \quad (\mathbf{w}\cdot\mathbf{n}_x)_e < 0 \end{cases} \qquad \phi_w = \begin{cases} \phi_W, & if \quad (\mathbf{w}\cdot\mathbf{n}_x)_w \geq 0 \\ \phi_P, & if \quad (\mathbf{w}\cdot\mathbf{n}_x)_w < 0 \end{cases}$$

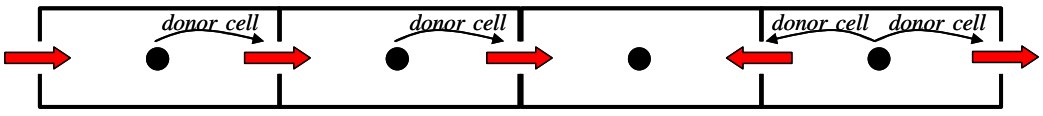
$$\phi_n = \begin{cases} \phi_P, & if \quad (\mathbf{w}\cdot\mathbf{n}_y)_n \geq 0 \\ \phi_N, & if \quad (\mathbf{w}\cdot\mathbf{n}_y)_n < 0 \end{cases} \qquad \phi_s = \begin{cases} \phi_S, & if \quad (\mathbf{w}\cdot\mathbf{n}_y)_s \geq 0 \\ \phi_P, & if \quad (\mathbf{w}\cdot\mathbf{n}_y)_s < 0 \end{cases}$$

  this translates the already observed concept seen in the 1D case for the advection equation **and results in a first order accurate scheme that is rather *"diffusive"* (see above), i.e. rather affected by truncation error;**

  Concerning the upwind difference scheme, it must be noted that *this technique is frequently used in system codes for two-phase flow and takes the name of "donor cell principle"*

In particular, in this case the concept of *volumes* and *junctions* separating them is mostly *like the Eulerian lumped parameter approach consisting in subdividing a system into "rooms" separated by "doors"*:

- ***in each room (volume), mass and energy balance equations are solved*** **to specify the thermodynamic properties of the fluid being inside**
- ***across each door (junction), momentum equations are solved*** **to specify the inlet and outlet flows**



With such a simplified model in mind, it is spontaneous to introduce a simple rule for evaluating the properties of the inlet and outlet flows in terms of the properties in the *"uspstream"* volume (i.e., the *"donor cell"*). Such a rule, translates into control volume formulation the *"upwind differencing"* technique seen for the advection equation.

- ***linear interpolation (CDS):***

$$\phi_e = (1-\lambda_e)\phi_P + \lambda_e \phi_E \qquad\qquad \lambda_e = \frac{x_e - x_P}{x_E - x_P} \qquad \textbf{ecc.}$$

in this case, we have a second order accurate scheme, but oscillatory behaviour may be observed, as it is usual for *"centered difference schemes"*

- ***quadratic upwind interpolation (QUICK):***

$$\phi_e = \begin{cases} \phi_P + g_1(\phi_E - \phi_P) + g_2(\phi_P - \phi_W) & se \quad (\mathbf{w}\cdot\mathbf{n})_e \geq 0 \\ \phi_E + g_3(\phi_P - \phi_E) + g_4(\phi_E - \phi_{EE}) & se \quad (\mathbf{w}\cdot\mathbf{n})_e < 0 \end{cases}$$

with

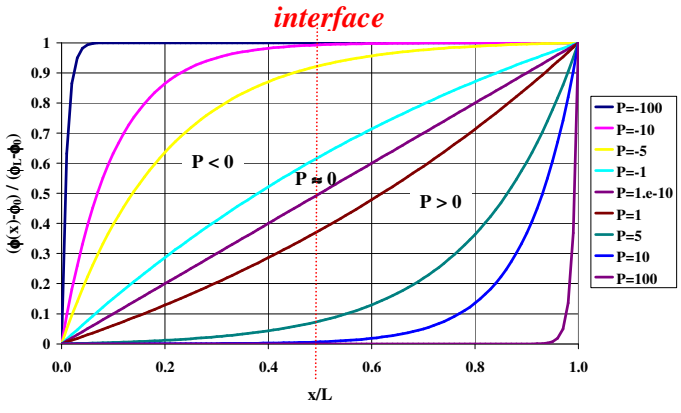
$$g_1 = \frac{(x_e - x_P)(x_e - x_W)}{(x_E - x_P)(x_E - x_W)} \qquad g_2 = \frac{(x_e - x_P)(x_E - x_e)}{(x_P - x_W)(x_E - x_W)}$$

$$g_3 = \frac{(x_e - x_E)(x_e - x_{EE})}{(x_P - x_E)(x_P - x_{EE})} \qquad g_4 = \frac{(x_e - x_E)(x_P - x_e)}{(x_E - x_{EE})(x_P - x_{EE})}$$

and similar formulations for the other directions; this scheme derives from *a parabolic interpolation combined with an "upwind" treatment*, providing a second order accurate scheme

- ***exponential, power law, hybrid scheme, etc.:***

S.V. Patankar, in "*Numerical Heat Transfer and Fluid Flow*" (1980) proposes a treatment based on the 1D steady-state advection-diffusion equation based on the consideration of a Peclet number, $P = \frac{\rho w}{\Gamma}\Delta x$, quantifying the ratio between advection and diffusion; on the basis of the exact solution and of the direction of motion, an exponential formulation and different approximations to it are proposed for the evaluation of the scalar at the interface



Finite Element Method (FEM)

The FEM is mostly based on the "weighted residual method" with a Galerkin weighting (see below) and has the following characteristics:

- ***the computational domain is discretised into "finite elements"*** **having sometimes complex shape**
- ***an approximating function is used for expressing the trend of the unknown variable in space*** **and it is expressed in terms of the value of the unknown variable in the "nodes" of the elements; for a steady state problem it is:**

$$\phi_{app}(x,y,z) = \sum_{i=1}^{N} \phi_i \varphi_i(x,y,z)$$

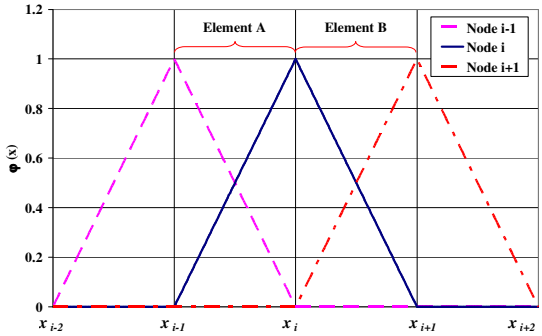
where ϕ_i are the nodal values;

- **the function $\varphi_i(x,y,z)$ are said *"trial functions"* (in the jargon of the method of weighted residuals) or *"shape functions"* (in the jargon of FEM); they are generally chosen among the low order polynomials, piecewise defined in contiguous elements**

The procedure for obtaining the discretised equations is composed of *two stages*.

<u>STAGE 1</u>: Piecewise interpolation

- ***It has the purpose to obtain the local solution expressed in terms of nodal values***
- **In one-dimensional cases it is possible to adopt *a linear interpolation***



e.g. for the element A in the figure it is

$$\varphi_i^A(x) = \frac{x - x_{i-1}}{x_i - x_{i-1}} \qquad \varphi_{i-1}^A(x) = \frac{x_i - x}{x_i - x_{i-1}} \qquad \textbf{with} \quad \varphi_{i-1}^A(x) + \varphi_i^A(x) = 1$$

obtaining the approximating functions in each element

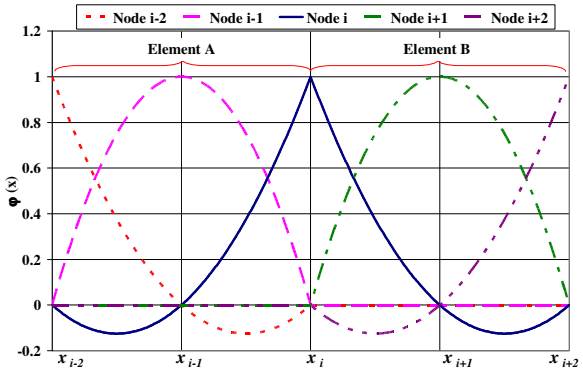
$$\phi^A(x)=\phi_{i-1}\varphi_{i-1}^A(x)+\phi_i\varphi_i^A(x) \qquad (x_{i-1}\le x\le x_i)$$

$$\phi^B(x)=\phi_i\varphi_i^B(x)+\phi_{i+1}\varphi_{i+1}^B(x) \qquad (x_i\le x\le x_{i+1})$$

- **Similarly, for *a quadratic interpolation***

$$\varphi_{i-2}^A(x)=\left(\frac{x-x_{i-1}}{x_{i-2}-x_{i-1}}\right)\left(\frac{x-x_i}{x_{i-2}-x_i}\right) \qquad \varphi_{i-1}^A(x)=\left(\frac{x-x_{i-2}}{x_{i-1}-x_{i-2}}\right)\left(\frac{x-x_i}{x_{i-1}-x_i}\right)$$

$$\varphi_i^A(x)=\left(\frac{x-x_{i-2}}{x_i-x_{i-2}}\right)\left(\frac{x-x_{i-1}}{x_i-x_{i-1}}\right) \quad \textbf{with} \quad \varphi_{i-2}^A(x)+\varphi_{i-1}^A(x)+\varphi_i^A(x)=1$$



in each element it is

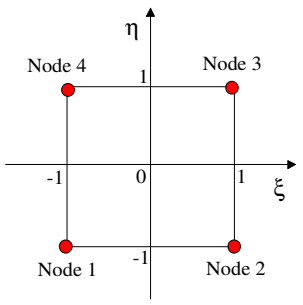
$$\phi^A(x)=\phi_{i-2}\varphi_{i-2}^A(x)+\phi_{i-1}\varphi_{i-1}^A(x)+\phi_i\varphi_i^A(x) \qquad (x_{i-2}\le x\le x_i)$$

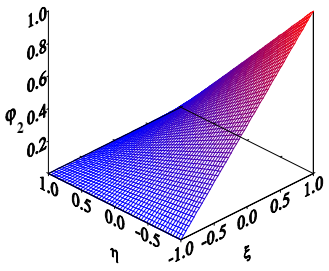
$$\phi^B(x)=\phi_i\varphi_i^B(x)+\phi_{i+1}\varphi_{i+1}^B(x)+\phi_{i+2}\varphi_{i+2}^B(x) \qquad (x_i\le x\le x_{i+2})$$

In 2D cases, it is possible to adopt *bi-linear* or *bi-quatratic interpolations*:

- ***bilinear***

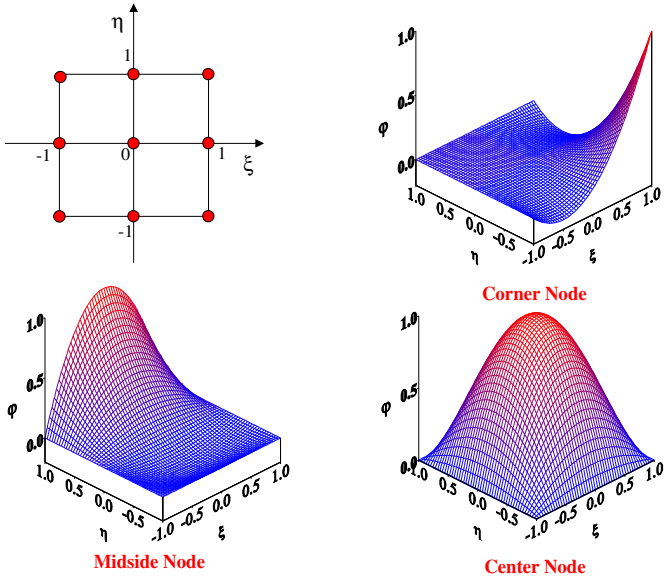
$$\begin{cases}\varphi_1(\xi,\eta)=0.25(1-\xi)(1-\eta)\\ \varphi_2(\xi,\eta)=0.25(1+\xi)(1-\eta)\\ \varphi_3(\xi,\eta)=0.25(1+\xi)(1+\eta)\\ \varphi_4(\xi,\eta)=0.25(1+\xi)(1-\eta)\end{cases} \qquad with \quad \sum_{i=1}^{4}\varphi_i(\xi,\eta)=1$$





- ***biquadratic***

$$\begin{aligned}
&\textit{Corner Nodes}: && \varphi_l(\xi,\eta) = 0.25\xi_l\xi(1+\xi_l\xi)\eta_l\eta(1+\eta_l\eta)\\
&\textit{Midside Nodes}\,(\xi_l = 0): && \varphi_l(\xi,\eta) = 0.5(1-\xi^2)\eta_l\eta(1+\eta_l\eta)\\
&\textit{Midside Nodes}\,(\eta_l = 0): && \varphi_l(\xi,\eta) = 0.5(1-\eta^2)\xi_l\xi(1+\xi_l\xi)\\
&\textit{Internal Node}: && \varphi_l(\xi,\eta) = (1-\xi^2)(1-\eta^2)
\end{aligned}$$



STAGE 2: Application of the weighted residual method

The weighted residual method represents *a general technique for approximating the solution of a partial differential equation*.

Let us assume that the differential equation is

$$L\phi = 0$$

with L an appropriate *differential operator*. As seen, an approximating function can be given by

$$\phi_{app}(x,y,z) = \sum_{i=1}^{N} c_i \varphi_i(x,y,z)$$

that should also satisfy the boundary conditions. The trial functions, $\varphi_i(x,y,z)$, can be chosen conveniently among different types of functions, though polynomials often preferred. As seen above, for a FEM the coefficients c_i should be the nodal values ϕ_i.

The *"residual"* of the equation, defined as

$$R(x,y,z) = L\phi_{app} \qquad (in\ general \neq 0)$$

will be obviously nonzero in general (unless ϕ_{app} is exact…); it must be minimised as far as possible. To obtain this result, different "weighting functions" $W_m(x,y,z)$ are defined, imposing *integral relationships* of the type

$$\int_V R(x,y,z,t) W_m(x,y,z)\, dV = \int_V L\phi_{app}(x,y,z,t) W_m(x,y,z)\, dV = 0$$

as many times as necessary to enable the calculation of the unknown coefficients c_i **(in our case ϕ_i). The algebraic equations obtained by this technique are *just the discretised equations in terms of the nodal values* i.e., *the equations of the numerical scheme*.**

Typical choices for the weighting functions are:

- **<u>Subdomain method</u>:** $$W_m = \begin{cases} 1, \ for\ \vec{r} \in V_m \\ 0, for\ \vec{r} \notin V_m \end{cases}$$

It is important to note that when the equation $L\phi = 0$ represents a conservation law, this imposes the integral conservation over V_m

$$\int_V L\phi_{app}(x,y,z,t) W_m(x,y,z)\, dV = \int_{V_m} L\phi_{app}(x,y,z,t)\, dV = 0$$

This requires that the approximate solution satisfy the integral balance on the volume as in finite volume methods.

- **<u>Collocation methods:</u>**

  In this case it is $W_m(\vec{r}) = \delta(\vec{r} - \vec{r}_m)$, with δ the Dirac's delta function

$$\int_V L\phi_{app}(\vec{r},t)\, \delta(\vec{r} - \vec{r}_m)\, dV = \left[L\phi_{app} \right](\vec{r}_m, t) = R(\vec{r}_m, t) = 0$$

  This requires that the residual vanishes at selected location in space

- **<u>Galerkin method</u>**

  In this case, the one mostly addressed with FEM, the *trial functions are used as weighting functions*: $W_m(\vec{r}) = \varphi_m(\vec{r})$

  It is interesting to note that when the trial functions form a complete basis, this implies that the residual should be orthogonal, in the sense of the scalar product between functions $(f,g) = \int_V f(\vec{r},t)\, g(\vec{r},t)\, dV$ at some element of the basis $\int_V R(\vec{r},t)\, \varphi_m(\vec{r})\, dV = 0 \ (m = 1,\ldots,M)$.

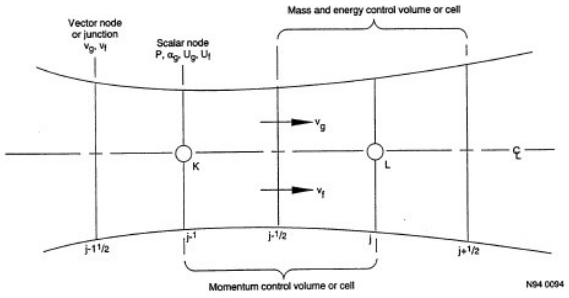
SOLVING COUPLED EQUATIONS

The need for pressure and velocity coupling

Due to the fact that sound speed is generally very large in compressible fluids and theoretically infinite in incompressible ones, *pressure perturbations travel very fast in the computational domain*

This gives rise to *the need to evaluate as far as possible implicitly the flow and the pressure fields*, *in order not to incur in a time step limitation similar to the one based on the Courant number, but evaluated with the sound speed instead of the fluid one.*

In the "staggered mesh" scheme adopted by RELAP5, for instance, the *semi-implicit scheme* is conceived as follows:



- **the *linearised energy and mass balance equations in each control volume are combined*, with the aid of the *linearised state relationship*, to obtain *a link between node pressure and velocities at inlet and outlet junctions***

$$P_j^{n+1} = A\, v_{g,j+1/2}^{n+1} + B\, v_{g,j-1/2}^{n+1} + C\, v_{f,j+1/2}^{n+1} + D\, v_{f,j-1/2}^{n+1} + E$$

➢ ***owing to the pressure-velocity implicit link, momentum equations can be written in the form*** **(similar equations hold for the outlet junction)**

$$v_{g,j-1/2}^{n+1} = A^1(P_j^{n+1} - P_{j-1}^{n+1}) + C^1$$

$$v_{f,j-1/2}^{n+1} = B^1(P_j^{n+1} - P_{j-1}^{n+1}) + D^1$$

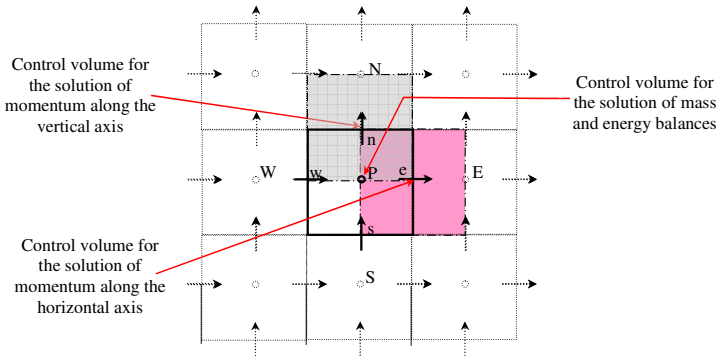
- ***Elimination of junction velocities*** **from these equations leads to *a sparse matrix system in the nodal pressures at the new time step***
- **For a simple pipe system with single inlet and outlet junctions, the algebraic system matrix is tridiagonal and the TDMA could be used; a sparse matrix solver is adopted for greater generality**

SIMPLE and SIMPLER Methods

In the case of CFD, this coupling between the pressure and the velocity fields is also needed to stabilise solutions

Considering the SIMPLE *(Semi-Implicit Method for Pressure-Linked Equations)* and SIMPLER *(SIMPLE Revised)* methods, two basic algorithms for the solution of mass and momentum coupled equations, help in clarifying this concept

With reference to a classical staggered mesh (not strictly required)



the momentum equations are written in control volume formulation

$$\underbrace{\frac{d}{dt}\int_V \rho\, w_x dV}_{\text{rate of change}} + \underbrace{\int_S w_x \left(\rho\, \vec{w}\cdot\vec{n}\right) dS}_{\text{advection term}} = \underbrace{\int_S f_{\tau,x}\, dS}_{\text{viscous forces}} - \underbrace{\int_S p n_x\, dS}_{\text{pressure force}} + \underbrace{\int_V \rho\, g_x\, dV}_{\text{body force}}$$

$$\underbrace{\frac{d}{dt}\int_V \rho\, w_y dV}_{\text{rate of change}} + \underbrace{\int_S w_y \left(\rho\, \vec{w}\cdot\vec{n}\right) dS}_{\text{advection term}} = \underbrace{\int_S f_{\tau,y}\, dS}_{\text{viscous forces}} - \underbrace{\int_S p n_y\, dS}_{\text{pressure force}} + \underbrace{\int_V \rho\, g_y\, dV}_{\text{body force}}$$

Volume and surface integrals are written in appropriate forms, according to the finite volume technique, *paying attention to point out the link between the net pressure difference along each axis and the related velocities*. For instance at the boundary "*e*" (see the above figure) the x-velocity is linked to the pressure difference in the adjoining volumes as

$$a_e w_{x,e} = \sum_{nb} a_{nb} w_{x,nb} + b + \left(p_P - p_E\right) A_e$$

where *nb* means "neighbouring" and indicates the contribution to the momentum change coming from the adjoining nodes

In this equation:

- a_{nb} ***accounts for the advective and diffusive contributions*** **from the adjoining (neighbouring) nodes;**
- b ***is a general source term*** **for body force and all the other terms evaluated explicitly (it will be repeated in the following equations with similar meaning <u>but different actual value</u>)**
- $(p_P - p_E)A_e$**, represents the net of pressure forces over the control volume for momentum along the horizontal axis;** ***it can be noted as the staggered mesh arrangement allows for the direct use of nodal pressures in P and E to represent the pressure difference across the interface***
- A_e **represents <u>the lateral area</u> on which the pressure force acts**

The fact to have singled out the pressure difference term in the equations will allow evaluating <u>*in a coupled way*</u> the pressure and velocity fields

Momentum equation along the y-axis has a similar form

$$a_n w_{y,n} = \sum_{nb} a_{nb} w_{y,nb} + b + (p_P - p_N)A_n$$

Whenever a third axis is present, an additional equation for the related component will appear

$$a_t w_{z,t} = \sum_{nb} a_{nb} w_{z,nb} + b + (p_P - p_T)A_t$$

Since the pressure field at the new time step is not yet known, it is necessary to make use of *an estimate of pressure* (indicated with a *) that will provide velocities that, in general, will not satisfy continuity

A guessed velocity field will be then obtained **by solving momentum equations**

$$a_e w^*_{x,e} = \sum_{nb} a_{nb} w^*_{x,nb} + b + (p^*_P - p^*_E)A_e$$

$$a_n w^*_{y,n} = \sum_{nb} a_{nb} w^*_{y,nb} + b + (p^*_P - p^*_N)A_n$$

$$a_t w^*_{z,t} = \sum_{nb} a_{nb} w^*_{z,nb} + b + (p^*_P - p^*_T)A_t$$

Since the velocity field does not satisfy continuity it will be necessary to introduce a *velocity correction* (primed quantities) that will result in a corresponding *pressure correction*:

$$p = p^* + p' \qquad w_x = w_x^* + w_x' \qquad w_y = w_y^* + w_y' \qquad w_z = w_z^* + w_z'$$

Subtracting side by side the following equations

$$a_e w_{x,e} = \sum_{nb} a_{nb} w_{x,nb} + b + \left(p_P - p_E\right) A_e \qquad a_e w_{x,e}^* = \sum_{nb} a_{nb} w_{x,nb}^* + b + \left(p_P^* - p_E^*\right) A_e$$

the equation for the corrections is obtained

$$a_e w_{x,e}' = \sum_{nb} a_{nb} w_{x,nb}' + \left(p_P' - p_E'\right) A_e$$

In the SIMPLE algorithm it is therefore assumed that *the first term at the RHS can be neglected*. This approximation will be corrected in the SIMPLER scheme.

By adopting such simplification, it is

$$a_e w_{x,e}' \approx \left(p_P' - p_E'\right) A_e$$

and we write

$$w_{x,e}' = d_e \left(p_P' - p_E'\right) \qquad d_e \equiv A_e / a_e$$

The velocity correction formulations are then obtained:

$$w_{x,e} = w_{x,e}^* + d_e \left(p_P' - p_E'\right) \qquad w_{y,n} = w_{y,n}^* + d_n \left(p_P' - p_N'\right) \qquad w_{z,t} = w_{z,t}^* + d_t \left(p_P' - p_T'\right)$$

Of course, similar relationships must be defined over the remaining faces of the control volume

$$w_{x,w} = w_{x,w}^* + d_w \left(p_W' - p_P'\right) \qquad w_{y,s} = w_{y,s}^* + d_s \left(p_S' - p_P'\right) \qquad w_{z,b} = w_{z,b}^* + d_b \left(p_B' - p_P'\right)$$

In order to find an equation for the corrections, *use is made of the continuity equation*. In fact, it is clear that, in addition to satisfy the momentum equations along the three axes, *the velocity field must satisfy the compressible or incompressible continuity equations*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{w}\right) = 0 \qquad \nabla \cdot \vec{w} = 0$$

(in the latter case a "divergence-free" velocity field is obtained).

***Either equation leads to a constraint in pressure that is named "Poisson equation",* as the classical equation of Electromagnetism**

For the general case of a *compressible fluid*, the equation

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho\vec{w})=\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x}(\rho w_x)+\frac{\partial}{\partial y}(\rho w_y)+\frac{\partial}{\partial z}(\rho w_z)=0$$

takes the space and time discretised form

$$\frac{(\rho_P-\rho_P^0)\Delta x\Delta y\Delta z}{\Delta t}+\left[(\rho w_x)_e-(\rho w_x)_w\right]\Delta y\Delta z+\left[(\rho w_y)_n-(\rho w_y)_s\right]\Delta x\Delta z+\left[(\rho w_z)_t-(\rho w_z)_b\right]\Delta x\Delta y=0$$

(all the terms are evaluated <u>at the new time step</u>, except the one with the 0 superscript, evaluated at the previous one)

Substituting in this equation the formulas for velocity obtained by momentum equation, including corrections, we have the *Poisson equation*

$$a_P p'_P=a_E p'_E+a_W p'_W+a_N p'_N+a_S p'_S+a_T p'_T+a_B p'_B+b$$

representing a 7 point equation (or 5 point in 2D o 3 point in 1D), where

$$a_E=\rho_e d_e\Delta y\Delta z \qquad a_W=\rho_w d_w\Delta y\Delta z \qquad a_N=\rho_n d_n\Delta x\Delta z \qquad a_S=\rho_s d_s\Delta x\Delta z$$

$$a_T=\rho_t d_t\Delta x\Delta y \qquad a_B=\rho_b d_b\Delta x\Delta y$$

$$a_P=a_E+a_W+a_N+a_S+a_T+a_B$$

$$b=\frac{(\rho_P^0-\rho_P)\Delta x\Delta y\Delta z}{\Delta t}+\left[(\rho w_x^*)_w-(\rho w_x^*)_e\right]\Delta y\Delta z+\left[(\rho w_y^*)_s-(\rho w_y^*)_n\right]\Delta x\Delta z+\left[(\rho w_z^*)_b-(\rho w_z^*)_t\right]\Delta x\Delta y$$

In relation to the above, it can be pointed out that:

- ***it is quite evident the analogy with the semi-implicit numerical scheme adopted by RELAP5* that, in the case of a 1D pipe, gives rise to *a three-point equation in nodal pressures*: the pressure-velocity coupling procedure is basically the same**
- **since the values $\rho_e,\rho_w,ecc.$ are not immediately available, since the scalar quantities are evaluated in the nodes P, E, W, etc., it is then necessary to interpolate putting particular attention to *make use of the same density value for both the control volumes adjoining the interface***

this is a fundamental requirement
to maintain the conservation property in the scheme

- **the *b* coefficient is nothing but *a residual of the continuity equation based on the guessed (starred) velocities*: monitoring its decrease during iterations will give an idea about convergence**

On the basis of the above formulations, the algorithm proceeds as follows:

1. **an estimate of the pressure field p^* is assigned;**
2. **momentum equations are solved;**

$$a_e w^*_{x,e} = \sum_{nb} a_{nb} w^*_{x,nb} + b + \left(p^*_P - p^*_E\right)A_e \qquad a_w w^*_{x,w} = \sum_{nb} a_{nb} w^*_{x,nb} + b + \left(p^*_W - p^*_P\right)A_w$$

$$a_n w^*_{y,n} = \sum_{nb} a_{nb} w^*_{y,nb} + b + \left(p^*_P - p^*_N\right)A_n \qquad a_s w^*_{y,s} = \sum_{nb} a_{nb} w^*_{y,nb} + b + \left(p^*_S - p^*_P\right)A_s$$

$$a_t w^*_{z,t} = \sum_{nb} a_{nb} w^*_{z,nb} + b + \left(p^*_P - p^*_T\right)A_t \qquad a_b w^*_{z,b} = \sum_{nb} a_{nb} w^*_{z,nb} + b + \left(p^*_B - p^*_P\right)A_b$$

3. **the system of equations for p' is solved:**

$$a_P p'_P = a_E p'_E + a_W p'_W + a_N p'_N + a_S p'_S + a_T p'_T + a_B p'_B + b$$

4. **the corrected pressures are calculated:**

$$p = p^* + p'$$

5. **the corrected values of velocities are calculated:**

$$w_{x,e} = w^*_{x,e} + d_e\left(p'_P - p'_E\right) \qquad w_{y,n} = w^*_{y,n} + d_n\left(p'_P - p'_N\right) \qquad w_{z,t} = w^*_{z,t} + d_t\left(p'_P - p'_T\right)$$

$$w_{x,w} = w^*_{x,w} + d_w\left(p'_W - p'_P\right) \qquad w_{y,s} = w^*_{y,s} + d_s\left(p'_S - p'_P\right) \qquad w_{z,b} = w^*_{z,b} + d_b\left(p'_B - p'_P\right)$$

6. **all the other balance equations are solved (energy, concentration, turbulence parameters, etc.) in case in which they may affect the velocity field**
7. **the new value of p is taken as the new estimate p^* and the process continues from step 2 until convergence is reached.**

Notes:

- **Sometimes in order to avoid problems in convergence, *under-relaxation is necessary in the calculation of pressures*:**

$$p = p^* + \alpha_p p'$$

appropriate values of α_p are generally between 0.5 e 0.8.

- **The *boundary conditions* to be imposed in pressure correction equations may be of two types:**
  - **wherever pressure is imposed, it is always $p' = 0$, since pressure is known, and the number of unknowns is decreased by one;**
  - **wherever velocity is imposed, this does not depend on pressure: the number of unknowns is again decreased by one.**

- **When an incompressible fluid is considered, since there is no link between pressure and fluid properties (density), in the momentum balance equation there is nothing allowing to determine the pressure magnitude:**

what matters are only the differences in pressure,
that has therefore a relative character

- **This relative character of pressure actually makes indeterminate the linear system for pressure correction; however:**
  - **this does not constitute a problem for iterative solvers, since the initialization of the solution will drive convergence towards a specific solution**
  - **in the case of a direct solution method, it is necessary to assign an arbitrary value of p' in any place, thus making determinate the system of equations.**

In the SIMPLER algorithm, the neglect of the term $\sum_{nb} a_{nb} w'_{x,nb}$ in pressure correction equations is avoided *since it leads to an overestimate of the correction, requiring under-relaxation*.

To improve convergence, momentum balance equations

$$a_e w_{x,e} = \sum_{nb} a_{nb} w_{x,nb} + b + (p_P - p_E) A_e$$

are reconsidered writing them in the form

$$w_{x,e} = \frac{\sum_{nb} a_{nb} w_{x,nb} + b}{a_e} + (p_P - p_E)\frac{A_e}{a_e} = \frac{\sum_{nb} a_{nb} w_{x,nb} + b}{a_e} + (p_P - p_E) d_e$$

A pseudo-velocity is thus introduced

$$\hat{w}_{x,e} = \frac{\sum_{nb} a_{nb} w_{x,nb} + b}{a_e}$$

obtaining an equation in the form

$$w_{x,e} = \hat{w}_{x,e} + \left(p_P - p_E \right) d_e$$

This equation is similar to

$$w_{x,e} = w^*_{x,e} + d_e \left(p'_P - p'_E \right)$$

adopted in SIMPLE, but $\hat{w}_{x,e}$ **takes the place of** $w^*_{x,e}$ **and pressures** p **take the place of** p'**.**

A Poisson equation is therefore written in terms of pressures p**:**

$$a_P p_P = a_E p_E + a_W p_W + a_N p_N + a_S p_S + a_T p_T + a_B p_B + b$$

where

$$b = \frac{\left(\rho_P^0 - \rho_P \right) \Delta x \Delta y \Delta z}{\Delta t} + \left[\left(\rho \hat{w}_x \right)_w - \left(\rho \hat{w}_x \right)_e \right] \Delta y \Delta z$$

$$+ \left[\left(\rho \hat{w}_y \right)_s - \left(\rho \hat{w}_y \right)_n \right] \Delta x \Delta z + \left[\left(\rho \hat{w}_z \right)_b - \left(\rho \hat{w}_z \right)_t \right] \Delta x \Delta y$$

The steps in SIMPLER are therefore the following:

1. **guess the velocity field;**
2. **evaluate the coefficients in the momentum balance equations and the pseudo-velocities** $\hat{w}_{x,e}$

$$\hat{w}_{x,e} = \frac{\sum_{nb} a_{nb} w_{x,nb} + b}{a_e}$$

3. **the coefficients are calculated for the pressure equation**

$$a_P p_P = a_E p_E + a_W p_W + a_N p_N + a_S p_S + a_T p_T + a_B p_B + b$$

   which is then solved

4. **then the obtained pressure field is treated as an estimated pressure field** p^* **and the corresponding velocities** $w^*_{x,e}$ **and similar are calculated**

$$a_e w^*_{x,e} = \sum_{nb} a_{nb} w^*_{x,nb} + b + \left(p^*_P - p^*_E \right) A_e \qquad a_w w^*_{x,w} = \sum_{nb} a_{nb} w^*_{x,nb} + b + \left(p^*_W - p^*_P \right) A_w$$

$$a_n w^*_{y,n} = \sum_{nb} a_{nb} w^*_{y,nb} + b + \left(p^*_P - p^*_N\right)A_n \qquad a_s w^*_{y,s} = \sum_{nb} a_{nb} w^*_{y,nb} + b + \left(p^*_S - p^*_P\right)A_s$$

$$a_t w^*_{z,t} = \sum_{nb} a_{nb} w^*_{z,nb} + b + \left(p^*_P - p^*_T\right)A_t \qquad a_b w^*_{z,b} = \sum_{nb} a_{nb} w^*_{z,nb} + b + \left(p^*_B - p^*_P\right)A_b$$

5. **the quantity**

$$b = \frac{\left(\rho^0_P - \rho_P\right)\Delta x\Delta y\Delta z}{\Delta t} + \left[\left(\rho\hat{w}_x\right)_w - \left(\rho\hat{w}_x\right)_e\right]\Delta y\Delta z + \left[\left(\rho\hat{w}_y\right)_s - \left(\rho\hat{w}_y\right)_n\right]\Delta x\Delta z + \left[\left(\rho\hat{w}_z\right)_b - \left(\rho\hat{w}_z\right)_t\right]\Delta x\Delta y$$

is calculated and the pressure equation is solved p':

$$a_P p'_P = a_E p'_E + a_W p'_W + a_N p'_N + a_S p'_S + a_T p'_T + a_B p'_B + b$$

6. **the velocity field is corrected:**

$$w_{x,e} = w^*_{x,e} + d_e\left(p'_P - p'_E\right) \qquad w_{y,n} = w^*_{y,n} + d_n\left(p'_P - p'_N\right) \qquad w_{z,t} = w^*_{z,t} + d_t\left(p'_P - p'_T\right)$$

$$w_{x,w} = w^*_{x,w} + d_w\left(p'_W - p'_P\right) \qquad w_{y,s} = w^*_{y,s} + d_s\left(p'_S - p'_P\right) \qquad w_{z,b} = w^*_{z,b} + d_b\left(p'_B - p'_P\right)$$

<u>but pressures are not corrected</u>

7. **balance equations for the other variables are solved (energy, concentration, turbulence parameters, etc.) if needed**
8. **the algorithm is repeated from step 2 until convergence is reached.**

<u>Notes:</u>

- **One of the main differences between SIMPLE and SIMPLER is that the latter does not make use of an estimated pressure field but only of an estimated velocity field; the pressure field is calculated on the basis of the velocity field**

- **When the velocity field reaches convergence, the pressure field will be the correct one**

- **The SIMPLER converges more rapidly than SIMPLE, *but the computational effort per iteration is larger*; the overall result is anyway generally in favour of SIMPLER**